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COMBUSTION RESEARCH BULLETIN

No. 121 June 2001

A News Bulletin of the Office of Basic Energy Sciences, Department of Energy, Combustion Research Programs. Produced by Keith Schofield, ChemData Research, P.O. Box 40481, Santa Barbara, CA 93140, (805) 966-7768, Fax (805) 893-8797, e-mail: combust@mrl.ucsb.edu, http://www.ca.sandia.gov/CRF/Publications/CRB/CRB.html

TECHNICAL ABSTRACTS

DROPLET COMBUSTION CONTROL FOR MICROGRAVITY EXPERIMENTS

R. Lobbia, S. Dattarajan, O.I. Smith and A.R. Karagozian, University of California at Los Angeles (Presented at the *54th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in San Diego CA, November 2001).

This experimental study focuses on development of a method for performing sustained droplet combustion experiments via closed-loop control. The methodologies described here are especially pertinent in conducting microgravity droplet experiments, where the effects of perturbation conditions on droplet combustion behavior may be explored successively, over many seconds or even minutes, in a straightforward manner. In the present configuration, a burning liquid methanol droplet is suspended and maintained at a constant diameter during combustion via continuous fuel delivery through a quartz capillary tube. Both open loop and closed loop control of fuel delivery is explored in these studies, and the effect of continuous fuel delivery on droplet burning characteristics is examined.

DETERMINATION OF THE GAS TEMPERATURE IN AN OPEN AIR, ATMOSPHERIC PLASMA TORCH FROM THE RESOLVED PLASMA EMISSION

J.M. Williamson, Innovative Scientific Solutions, Inc., Dayton OH, C.A. Dejoseph, Jr., Air Force Research Laboratory, Wright-Patterson AFB, OH (Presented at the *54th Annual Gaseous Electronics Conference of the American Physical Society*, Held in University Park PA, October 2001).

In principle, the gas temperature in an air plasma can be determined from the plasma emission of molecular nitrogen. The gas temperature is typically determined from the contour analysis of the emission bands in the well known, N_2 2nd positive ($C^3\Pi$-$B^3\Pi$) system. The N_2 2nd positive system has a large oscillator strength and is easily recognized in nitrogen discharges making it the preferred system for temperature determination. The resolved emission spectrum of an atmospheric pressure, open-air plasma torch was recorded with a 0.5 m spectrometer and CCD camera. The plasma emission under these conditions was found to be dominated by continuum radiation and emission from other species which obscured large portions of the N_2 2nd positive emission. In spite of these difficulties, the gas temperature of the torch could be determined from a fit of partially resolved N_2^+ 1st negative vibrational transitions and a blackbody fit to the continuum radiation. The vibrational temperature, determined from a Boltzmann plot, was 4300(±900) K while the blackbody radiation temperature was 4400(±400) K. As a check, spectral simulations using N_2^+ 1st negative emission, N_2 2nd positive emission, and a blackbody were compared with measured spectra over selected spectral regions.

STUDY OF INTENSITY DISTRIBUTION IN THE R(0,0) BRANCH OF THE ($A^1P \circledR X^1S^+$) ELECTRONIC TRANSITION OF THE BH MOLECULE AND DETERMINATION OF GAS TEMPERATURE IN NON-EQUILIBRIUM PLASMAS

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Relative transition probabilities of spontaneous emission in the R and P branches of the ($A^1\Pi$-$X^1\Sigma^+$), (0,0) band of BH have been obtained for the first time. It was observed that they are in agreement to corresponding ratios of Honl-London factors. Thus the nonadiabatic effect of perturbation is negligibly small and Honl-London formulas may be used for derivation of rovibronic population densities from measured line intensities. General considerations are illustrated by the example of a low-pressure plasma of a planar microwave discharge using H_2/Ar/B_2H_6 gas mixture (1-2.5 mbar, 1.2-2.4 kW). In the framework of a corona model the rotational temperatures of $A^1\Pi^-$, $v'=0$, and $X^1\Sigma^+$, $v''=0$ vibronic states obtained from the BH spectrum are in accordance with the rotational temperatures of the $X^1\Sigma^+$, $v''=0$ state of H_2 determined from the intensities of Q-branch (0,0) lines of the H_2-Fulcher-α band system. This provides the opportunity to use rotational line intensities of the R branch (0,0) of BH for the spectroscopic determination of rotational and gas temperatures in non-equilibrium plasmas.

ROTATIONAL TEMPERATURE MEASUREMENTS IN A RADIOFREQUENCY DISCHARGE BY USING CO ROTATIONAL EMISSION SPECTRUM

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Gas temperature is a necessary parameter needed to establish the kinetic model of a gas discharge. In order to verify the possible perturbation and distortion of temperature of the radiofrequency discharge to the thermocouple probe, we performed the emission spectroscopy analysis based on the rotational intensity distribution of CO bands to obtain highly accurate discharge temperature measurements. In our experiment, a well defined gas mixture with 95% of CO_2 and pressure 4-6 torr flowed transversely to the applied radiofrequency field between two parallel circular stainless steel disks with diameters of 2.54 cm and a discharge gap of 0.4-1.0 cm. The driven radiofrequency field had the frequency of 20-40 MHz and the power delivered to discharge was 1-5 W. It was possible in this discharge condition to use the Angstrom Band ($B^1\Sigma^+$-$A^1\Pi$, 519.8, 451.0 nm) in the visible emission spectrum of CO to analyze the discharge temperature. The Q branch within ($B^1\Sigma^+$-$A^1\Pi$) transition, which corresponds to $\Delta J=3D_0$ and has the most intense distribution profile, was used to identify the rotational quantum numbers. The higher rotational quantum numbers were used during the fitting in order to eliminate the possible overlap with P and R branches. The rotational temperature of the radiofrequency discharge in the gas mixture was compared to the temperature measured by thermocouple probe.

THOMSON SCATTERING MEASUREMENT OF ELECTRON DENSITY AND TEMPERATURE IN A MICROWAVE PLASMA FOR DIAMOND DEPOSITION

S. Narishige, S. Kitamura, K. Teii, K. Uchino and K. Muraoka, Kyushu University, Japan, and T. Sakoda, Kitakyushu National College Technology, Japan (Presented at the *54th Annual Gaseous Electronics Conference of the American Physical Society*, Held in University Park PA, October 2001).

The composition and flux of gaseous species in a reactive plasma are highly affected by the behavior of electrons. The detection of electrons in a microwave plasma operating at pressures as high as 10-100 torr is known to be difficult. For example, the small mean-free path obstructs the use of electrostatic probes. In this study, electron density (n_e) and temperature (T_e) in a microwave CH_4/H_2 plasma for diamond deposition were measured by laser Thomson scattering spectroscopy. This method can provide the local density and temperature without perturbing the discharge condition. A Nd:YAG laser at a frequency doubled wavelength of 532 nm was injected into the chamber. The scattered light was passed through a double-monochromator and the output signal was detected by a photomultiplier tube. With a pure H_2 plasma at 20 torr, $n_e=3x10^{17}$ m^{-3} and $T_e=1.7$ eV were obtained. However, with a 10% CH_4/90%H_2 plasma, the scattering spectrum confirmed that the component of rotational Raman scattering of molecules originated from CH_4 were overlapped on the Thomson scattering spectrum. It was found that the use of a Nd:YAG laser at fundamental wavelength of 1064 nm was suitable to suppress the component of the Raman scattering since the scattering intensity is inversely proportional to the 4th power of wavelength.

EFFECTS OF IGNITION ON PREMIXED VORTEX RINGS: A SIMULTANEOUS PLIF AND PIV INVESTIGATION

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Preliminary studies of reacting, premixed vortex rings have shown that flame propagation is highly sensitive to ignition timing, equivalence ratio, and vortex strength. A variety of divergent phenomena have been observed, such as interior/exterior flame propagation, vortex-induced flame bridging across the jet column, and the formation of unburned pockets. In the current work, planar laser induced fluorescence of acetone and OH is performed to study the non-reacting and reacting regions, respectively, and particle image velocimetry is used to study the effects of reaction on the flowfield. The flowfield consists of well-characterized vortex rings of premixed methane and air generated at the exit of an axisymmetric nozzle using a solenoid-driven piston. Ignition is initiated at various phases of vortex development and propagation. Results are compared with corresponding numerical simulations from a time-dependent computational fluid dynamics code with chemistry.

A NEW MODEL OF FLAMES AS GASDYNAMIC DISCONTINUITIES

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In premixed combustion a fresh mixture reacts to form lighter products. The first model of a flame as a discontinuity surface was due to Darrieus and to Landau. We propose a new model which replaces the thin flame region in which the fluid variables change continuously, and in which chemical reactions and diffusive processes occur, by a surface of discontinuity across which the fluid variables jump. We derive new expressions for the flame speed and the jump conditions, which provide corrections to previous expressions, and interpret them in terms of simple physical concepts. Compressibility is accounted for by appropriate surface forces. In contrast to previous models our conditions provide for the cutoff of the growth of all short wave perturbations, thus making the model more useful for both analytical and numerical considerations.

LATTICE BOLTZMANN ALGORITHM FOR LAMINAR JET DIFFUSION FLAME

T. Lee, C.-L. Lin and L.-D. Chen, Department of Mechanical Engineering, the University of Iowa (Presented at the *54th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in San Diego CA, November 2001).

A two-distribution lattice Boltzmann algorithm is presented to solve the Burke-Schumann diffusion flame. One distribution function represents the transport of the Schwab-Zeldovich coupling function, viz, the mixture fraction that combines the energy and species equations. The other distribution function models the compressible Navier-Stokes equations. The modified equilibrium distribution functions recover the macroscopic governing equations up to second order accuracy. In order to capture large gradients near nozzle exit and simulate infinite domain, the characteristic-based Galerkin finite element method is used to discretize the set of lattice Boltzmann equations on unstructured mesh. In this study the flame for a slot burner is considered. The results are compared with benchmark experimental and numerical results.

MODEL-BASED INVESTIGATION OF CONTROL OF THERMOACOUSTIC INSTABILITY USING FLOW CONTROL
P. Mehta, M. Soteriou and A. Banaszuk, United Technologies Research Center (Presented at the *54th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in San Diego CA, November 2001).

Thermoacoustic instability in gas turbines and rockets develops when acoustic modes couple with unsteady heat release in a positive feedback loop. Heat release is concentrated in the shear layers behind bluff body flameholders or backward facing steps. The rate of mixing between fuel/air mixture and hot combustion products trapped in recirculation zones determines the phase between acoustic pressure and heat release oscillations. Control over the mixing rate would allow changing this phase, and thus possibly eliminating the positive feedback between heat release and pressure. We investigated an approach to breaking the heat release and acoustic coupling by enhancing or suppressing shear layer mixing with flow control using unsteady fluid dynamics models. To model the effect of acoustic waves and flow control on heat release, we developed a distributed, two-dimensional, unsteady, Lagrangian model for describing the combustion dynamics (including the flame propagation and shear layer evolution) behind a flameholder. From the distributed model we extracted a reduced-order frequency domain heat release model using forced response technique. We analyzed the coupled model involving acoustics and heat release and investigated effect of flow control on the amplitude of pressure oscillations.

STABILITY ENHANCEMENT OF LEAN, PREMIXED FLAMES BY FLAMEHOLDER HEATING
J.C. Hermanson and N. Demmons, Worcester Polytechnic Institute (Presented at the *54th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in San Diego CA, November 2001).

The effects of flameholder heating on the stability and emissions of lean, premixed, turbulent flames were examined experimentally. The flames were stabilized by an axial, cylindrical bluff-body flameholder 6.4 mm in diameter made of copper or stainless steel. In some cases, the stainless flameholder was heated electrically. The flame was at atmospheric pressure. The premixed ethylene/air mixture upstream of the flameholder was unheated and had an equivalence ratio of 0.37 to 0.87. The cold gas flow velocities ranged from 5.0 to 10.5 m/s to give Reynolds numbers at the flameholder tip from 3250 to 6700. The impact of flameholder heating on the lean blow-off limit was determined visually. Heating the flameholder to yield a local mixture temperature of 190 °C resulted in a decrease in the equivalence ratio at lean blow-off of approximately 20%. This decrease in equivalence ratio resulted in up to a 26% decrease in exhaust-plane NO_x emissions and a 51 K reduction in the exhaust-plane gas temperature. These reductions were consistent with the lower equivalence ratios attainable by the localized mixture preheating. At the same time, the exhaust concentrations of CO and unburned hydrocarbons increased by a factor of approximately two. A smaller increase in lean flame stability was seen for the unheated stainless flameholder versus the copper flameholder.

EFFECT OF TURBULENCE INTENSITY ON METHANE/AIR TURBULENT PREMIXED FLAMES
M. Tanahashi, T. Saito and T. Miyauchi, Department of Mechanical and Aerospace Engineering, Tokyo Institute of Technology (Presented at the *54th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in San Diego CA, November 2001).

Direct numerical simulations (DNS) of methane/air turbulent premixed flames propagating in two-dimensional homogenous isotropic turbulent are conducted. Temperature dependence transport and thermal properties and detailed kinetic mechanism including 279 elementary reactions and 49 reactive species; that is GRImech 2.11., are considered to simulate methane/air premixed flames in turbulence. To clarify the effect of turbulence intensity, DNS are conducted for the cases of turbulence intensity (u_{rms}/S_L) of 10, 20 and 30 under the constant turbulence length scale. The local flame elements in turbulence are identified by using local maximum of temperature gradients and statistics of turbulent premixed flames are investigated. These statistics are compared with the previous study of hydrogen/air turbulent premixed flames with same turbulence intensity and scale. Additionally, a NO_x formation mechanism in turbulent premixed flame is investigated.

FULLY MODULATED TURBULENT DIFFUSION FLAMES IN MICROGRAVITY
R. Sangras, J.C. Hermanson and H. Johari, Worcester Polytechnic Institute, and D.P. Stocker and U.G. Hegde, NASA Glenn Research Center (Presented at the *54th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in San Diego CA, November 2001).

Fully modulated, turbulent diffusion flames are studied in microgravity in 2.2 s drop-tower tests with a coflow combustor. The fuel consists of pure ethylene or a 50/50 mixture with nitrogen; the oxidizer is either normal air or up to 40% oxygen in nitrogen. A fast solenoid valve is used to fully modulate (completely shut off) the fuel flow. The injection times range from 5 to 400 ms with a duty-cycle of 0.1-0.5. The fuel nozzle is 2 mm in diameter with a jet Reynolds number of 5000. The shortest injection times yield compact puffs with a mean flame length as little as 20% of that of the steady-state flame. The reduction in flame length appears to be somewhat greater in microgravity than in normal gravity. As the injection time increases, elongated flames result with a mean flame length comparable to that of a steady flame. The injection time for which the steady-state flame length is approached is shorter for lower air/fuel ratios. For a given duty-cycle, the separation between puffs is greater in microgravity than in normal gravity. For compact puffs, increasing the duty-cycle appears to increase the flame length more in microgravity than in normal gravity. The microgravity flame puffs do not exhibit the vortex-ring-like structure seen in normal gravity.

ACTIVE CONTROL OF MIXING AND COMBUSTION, FROM MECHANISMS TO IMPLEMENTATION
A.F. Ghoniem, Massachusetts Institute of Technology (Presented at the *54th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in San Diego CA, November 2001).

Implementation of active control in complex processes, of the type encountered in high Reynolds number mixing and combustion, is predicated upon the identification of the underlying mechanisms and the construction of reduced order models that capture their essential characteristics. The mechanisms of interest must be shown to be amenable to external actuations, allowing optimal control strategies to exploit the delicate interactions that lead to the desired outcome. Reduced order models are utilized in defining the form and requisite attributes of actuation, its relationship to the monitoring system and the relevant control algorithms embedded in a feedforward or a feedback loop. The talk will review recent work on active control of mixing in combustion devices in which strong shear zones concur with mixing, combustion stabilization and flame anchoring. The underlying mechanisms, for example stability of shear flows, formation/evolution of large vortical structures in separating and swirling flows, their mutual interactions with acoustic fields, flame fronts and chemical kinetics, etc., are discussed in light of their key roles in mixing, burning enhancement/suppression, and combustion instability. Subtle attributes of combustion mechanisms are used to suggest the requisite control strategies.

THE INTERACTION OF A FLAME WITH ITS SELF-INDUCED BOUNDARY LAYER

E.S. Oran, Naval Research Laboratory, J.D. Ott, University of Maryland, and J.D. Anderson, National Air and Space Museum (Presented at the *54th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in San Diego CA, November 2001).

The interactions of a boundary layer and a laminar flame, propagating from the closed to the open end of a small (order of centimeters) rectangular channel, were studied by solving the multdimensional, reacting, Navier-Stokes equations. As the flame propagates, boundary layers develop downstream of the flame. As the flame enters this boundary layer, burned material jets into the center of the channel. Whether the wall conditions are adiabatic or isothermal have a large effect on the impact of this jetting. When the walls are adiabatic, the flame velocity can increase by an order of magnitude within a short distance. When the walls are isothermal, energy losses at the walls induce a backward flow behind the flame. In this case, boundary material burns, jets into the channel, and then fountains both upstream and downstream. The flame alternatively accelerates and decelerates less and the flame velocity oscillates.

EXPLOITING IN SITU ADAPTIVE TABULATION (ISAT) TO SOLVE THE REACTIVE FLOW EQUATIONS

S.B. Pope and M.A. Singer, Cornell University (Presented at the *54th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in San Diego CA, November 2001).

We describe a novel second-order-accurate splitting scheme for reactive flows which exploits the ISAT algorithm to accelerate the computation of chemical reactions. This scheme offers substantial speed-up for applications such as the direct numerical simulation of turbulent combustion. The ISAT algorithm has previously been used to provide a thousandfold speed-up in the reaction sub-step in particle implementations of PDF methods. In order to use ISAT for the species conservation equations of reactive flows, it is necessary to split reaction into a sub-step separate from the other processes (i.e. convection and diffusion). A splitting scheme is presented and demonstrated which yields second-order accuracy in both space and time, even for very stiff systems and for time steps much larger than the smallest chemical timescales.

REDUCED KINETIC MECHANISMS IN NONPREMIXED FLAME-VORTEX INTERACTION

J. Hsu, Department of Mechanical Engineering, University of Colorado at Boulder, CO 80309, and S. Mahalingam, Department of Mechanical Engineering, University of California, Riverside, CA 92521 (Presented at the *54th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in San Diego CA, November 2001).

The goal of this work is to investigate the limits of applicability of progressively more accurate reduced kinetic schemes for methane/air flames using time dependence numerical simulations in a two-dimensional flow field. Nonpremixed one-, three and four-step reduced kinetic methane/air flame structure and flame response to interactions between a pair of counter-rotating vortices with an initially laminar unstrained flame is studied. Both continuous burning and localized extinction regimes that are consistent with the flamelet concept have been studied. A model to represent the quasi-steady extinction strain rate for various reduced kinetic mechanisms is proposed and validated.

SPINNING INSTABILITY OF GASEOUS DETONATIONS

A. Kasimov and D.S. Stewart, Theoretical and Applied Mechanics, University of Illinois, 216 Talbot Laboratory, 104 S. Wright St., Urbana, IL 61081 (Presented at the *54th Annual Meeting of the Division of Fluid Dynamics of the American Physical Society*, Held in San Diego CA, November 2001).

We investigate hydrodynamic instability of a steady planar detonation wave propagating in a circular tube to three-dimensional linear perturbations, using normal-mode approach. Spinning instability is identified and its relevance to the well-known spin detonation is discussed. The neutral stability curves in the plane of heat release and activation energy exhibit bifurcations from a single-head to multiple-head spinning modes as the heat release is increased at fixed activation energy. With a simple Arrhenius model for the heat release rate a remarkable qualitative agreement with experiment is obtained with respect to the effects of dilution, initial pressure, and tube diameter on the behavior of spin detonation. The analysis contributes to explanation of the spin detonation which has been lacking since the discovery of the phenomenon over seventy years ago.

Great Enhancements in Dissociative Electron Attachment to Chlorine Containing Molecules Adsorbed on H_2O/NH_3 Ice

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Dissociative electron attachment (DEA) to molecules in polar media may be an important process in the Earth's atmosphere and environment. We report that the presence of H_2O/NH_3 greatly enhances DEA of ~0 eV electrons to CF_2Cl_2, $CFCl_3$ and HCl molecules, respectively. The absolute DEA cross sections for these molecules adsorbed on H_2O/NH_3 ice are measured to be two to three orders of magnitude larger than those in the gas phase. This enhancement is due to the transfer of electrons trapped in the precursors of the fully solvated state in water or ammonia ice to chlorine-containing molecules that then dissociate. The results indicate that DEA to these ozone-depleting molecules adsorbed on polar stratospheric clouds under cosmic ray radiation is a very efficient process. The implication of this observation to atmospheric ozone depletion will be discussed.

Dynamics of Three-Body Dissociative Recombination of Dihydrides

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Dissociative recombination of triatomic dihydrides H_2D^+, CH_2^+, NH_2^+ and H_2O^+ show a large propensity for break-up into three atoms. The three-body yields for these cases ranges from 60 to 80%. In the cases of CH_2^+, NH_2^+ and OH_2^+, sufficient energy is released to yield the first excited electronic states of C, N and O. We determine the fraction going to the ground and excited states; the distribution of recoil energies; and the angular distribution of the two H atoms for each state of the center atom.

Recombination of H_3^+ and D_3^+ with Electrons: Low Limit of the Recombination Rate Coefficient

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From the decay of plasma in the mixture of He, Ar and H_2 (or D_2) we determined the overall rate constant (α) of the recombination of H_3^+ and D_3^+ ions with electrons. We observed pronounced dependence of α on partial pressure of hydrogen (deuterium). The dependence of α on the H_2 (or D_2) indicates that observed recombination proceeds most probably via formation of long lived Rydberg states that are stabilized against the reverse autoionization by collision with neutral molecule. From our study it follows that binary dissociative recombination of H_3^+ ions with electrons is very slow process (at 270 K) with a rate coefficient $\alpha < 3\times10^{-9}$ cm^3 s^{-1}.

ABSOLUTE CROSS SECTIONS FOR STATE SELECTED REACTIONS OF O^+ (^4S, ^2D, ^2P)

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We have obtained reliable absolute cross sections for the ion-molecule reactions $O^+(^4S, ^2D, ^2P) + N_2(H_2, CO_2, H_2O, O_2)$, which are recognized as the most important set of reactions in planetary ionospheres. A novel technique, which combines the radiofrequency octopole ion guide and the dissociative charge transfer reactions $He^+(Ne^+, Ar^+) + O_2$, has been successfully demonstrated and used for preparing state-selected reactant $O^+(^2P)$, $O^+(^2D)$, and $O^+(^4S)$ ions with high purities. We have also developed a differential retarding potential method for improving the center-of-mass kinetic energy ($E_{c.m.}$) resolution. These developments have made possible the measurement of absolute cross sections for the reactions involving state-selected $O^+(^4S,^2D,^2P)$ at kinetic energies down close to thermal energies. Notably, charge transfer product O_2^+ ions formed in the $O^+(^4S,^2D,^2P) + O_2$ reaction are known to undergo rapid dissociative recombination reactions with electrons, giving rise to excited oxygen atoms, which are the source of sky aurora.

PLASMA REMEDIATION OF NO_x IN THE PRESENCE OF HYDROCARBONS USING DIELECTRIC BARRIER DISCHARGES: MICROSTREAMER DISCHARGE DYNAMICS

R. Dorai and M.J. Kushner, University of Illinois (Presented at the *54th Annual Gaseous Electronics Conference of the American Physical Society*, Held in University Park PA, October 2001).

Plasma remediation is being investigated for removal of NO_x from automotive exhausts. Previous investigations using global kinetic models for simulated diesel exhausts containing N_2, O_2, CO_2, H_2O and ppm levels of NO, CO, H_2 and unburned hydrocarbons (UHCs) showed that the remediation process is primarily oxidative and most of the NO is converted to NO_2. In actual devices, the plasma consists of an assembly of filamentary microdischarges. The resulting nonuniformities in production rates of radicals and the depletion of feedstocks initiate convection which ultimately produces mixtures of reactants which are quantitatively different than uniform excitation. To study these processes, a radially dependent microdischarge model the plasma chemistry of simulated automotive exhaust, including UHCs, has been developed. The model includes a full accounting of the humid-air plasma chemistry, ambipolar charged particle transport and solution of the Navier-Stokes equations. Results will be discussed for the radial transport of reactive species and the consequences on NO_x remediation when including UHCs.

NO REMOVAL IN HIGH PRESSURE PLASMAS OF $N_2/H_2O/NO$ MIXTURES

F. Fresnet, G. Baravian, L. Magne, S. Pasquiers, C. Postel, V. Puech, A Rousseau, LPGP, Universit Paris-Sud/CNRS, France (Presented at the *54th Annual Gaseous Electronics Conference of the American Physical Society*, Held in University Park PA, October 2001).

Influence of H_2O on NO removal has been studied using a homogenous photo-triggered discharge with a time resolved LIF measurement of the NO density, in $N_2/H_2O/NO$ mixtures at 460 mbar. Measurement of NO density has been performed up to 180 s after the current pulse excitation of short duration, 50 ns. Kinetic analysis has been made using a self-consistent O-D discharge model. NO is in great part dissociated, in N_2/NO, through collisions with the excited singlet states of N_2. We have previously shown that addition of ethene induces de-excitation of these states, leading to a decrease of the NO removal. Similar processes take place when C_2H_4 is replaced by H_2O. The value of the rate constant for collision of singlet states with water, 3.10^{-10} cm^3 s^{-1}, is obtained from our study.

VIBRATIONALLY-MEDIATED DISSOCIATION OF H_2O MOLECULES INSIDE $(H_2O)_2$ AND Ar-H_2O COMPLEXES: SPECTROSCOPY, DYNAMICS, AND ALIGNMENT EFFECTS

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We observed the spectra of Ar-H_2O and $(H_2O)_2$ van der Waals complexes in the first OH stretching overtone ($2\nu_{OH}$) region using the technique of vibrationally mediated dissociation in a supersonic slit jet expansion. The complexes are first excited with a pulsed infrared OPO laser into a chosen rovibrational quantum state and then selectively photolyzed with an ultraviolet laser pulse. The choice of the intermediate state determines the specifics of the intramolecular vibrational motion as well as relative orientation of the complex's constituents prior to the photodissociation event. The OH fragments ejected as a result of photodissociation are interrogated with laser induced fluorescence. The OPO action spectra, which are obtained by scanning the infrared pump laser and keeping the probe laser fixed on an OH line, display a rich structure due to the presence of numerous vibrational bands attributable to H_2O, Ar-H_2O, $(H_2O)_2$ and quite possibly heavier complexes. Some bands display partial rotational resolution permitting an unambiguous assignment to a particular complex. Predissociation lifetimes (measured directly by varying the pump-photolysis delay) in the range of 10-50 ns are obtained for the Ar-H_2O(v=2) complex; $(H_2O)_2$ is found to predissociate in less than 5 ns. From the measured OH full quantum state distributions, detailed information is obtained on the photodissociation/vibrational predissociation dynamics of the Ar-H_2O and $(H_2O)_2$ complexes in the $2\nu_{OH}$ state.

RESONANCE ENHANCED DEACTIVATION OF Ar 4p¢[1/2]$_o$ STATE BY ATOMIC OXYGEN WITH IMPLICATIONS FOR Ar-BASED ACTINOMETRY

M. Brown, Innovative Scientific Solutions, Inc., Dayton, OH, B. Ganguly and A. Garscadden, Air Force Research Laboratory, Wright-Patterson AFB, OH (Presented at the *54th Annual Gaseous Electronics Conference of the American Physical Society*, Held in University Park PA, October 2001).

In SiC etching plasma devices, we have recorded plasma emission from Ar, F and O atoms in $SF_6/Ar/O_2$ radiofrequency discharges as a function of pressure, power and mixture fraction. In particular, we have examined Ar emission at 750 nm in comparison with Ar emission from other excited States. The excited state, 4p[1/2]$_o$(2p1), of the Ar 750 nm emission line is nearly iso-energetic with Rydberg states of atomic oxygen. We observed the resonant deactivation of this Ar excited state by O atoms in $SF_6/Ar/O_2$ radiofrequency driven discharges with high O_2 dissociation fractions. Using a variable gap and peak-to-peak voltage measurements, we estimated E/n to be 300 Td at 600 mtorr. For E/n>150 Td, 80 deposition in O_2 goes to dissociation. At fixed pressure and input power, the Ar emission at 750 nm decreases with O_2 additions up to 10[1/2]$_o$(3s5) Ar state at 641 nm increases with O_2 addition. The increased emission of the 641 nm line parallels that of F at 704 nm. The divergent behavior of the Ar emission lines is a manifestation of the resonant deactivation of the 4p[1/2]$_0$(2p1) state by O atoms which suggest the Ar 750 nm transition may not be suitable for actinometry in discharges containing oxygen and characterized by high E/n values.

INVESTIGATIONS IN FLUOROCARBON PLASMAS USING PLANAR LASER INDUCED FLUORESCENCE

K. Steffens, National Institute of Standards and Technology (Presented at the *54th Annual Gaseous Electronics Conference of the American Physical Society*, Held in University Park PA, October 2001).

Fluorocarbon plasmas are used within the semiconductor industry for processing applications including selective etching of SiO_2 and Si_3N_4, fabrication of MEMS structures, etching of low-k dielectrics, and post-CVD chamber-cleaning. The complex chemistry in fluorocarbon plasmas is dependent on many factors including precursor gas and plasma conditions. Although the mechanisms are still not completely understood, reactive radicals such as CF and CF_2 are known to be critical participants in the plasma chemistry. Measurements of these reactive species under a variety of relevant plasma conditions are important for gaining a better understanding of the plasma chemistry and to aid in process development and model validation. Planar laser induced fluorescence (PLIF) is a valuable tool for the measurement of two-dimensional maps of reactive species in plasmas. In this presentation, our most recent results using PLIF to measure reactive species distributions in fluorocarbon plasmas in the capacitively-coupled Gaseous Electronic Conference Radiofrequency Reference Cell will be discussed. A variety of plasma conditions have been investigated including different precursors, plasmas with and without a wafer present, and various pressures, plasma powers, and electrode gaps.

TALIF CALIBRATION WITH NOBLE GASES FOR QUANTITATIVE ATOMIC DENSITY MEASUREMENTS

K. Niemi, V. Schulz-Von der Gathen and H.F. Dobele, University of Essen, Germany, Institut fur Laser-und PlasmaPhysik Team (Presented at the *54th Annual Gaseous Electronics Conference of the American Physical Society*, Held in University Park PA, October 2001).

In order to obtain absolute atomic ground state densities with two-photon absorption laser induced fluorescence spectroscopy (TALIF), a reliable calibration technique and the consideration of collisional quenching effects on the induced population are required. A comparative measurement with a noble gas having a two-photon resonance spectrally close to the atomic transition can be used as a calibration. Suitable transitions exist in krypton and xenon for the two-photon excitation of atomic hydrogen at 205.1 nm, nitrogen at 206.6 nm, and oxygen at 225.5 nm. We investigated these excitations by TALIF in order to determine the atomic data required for this calibration. The radiative lifetimes of the excited states and the quenching coefficients for collisions with several important species were obtained from time resolved measurements. The relevant ratios of the two-photon excitation cross sections were determined from comparative measurements with known densities. The atomic reference densities were generated in a flow-tube reactor with the aid of titration methods.

INVESTIGATION OF THE $CN+C_2H_6$ AND $CN+CH_4$ EXOTHERMIC REACTIONS VIA STATE RESOLUTION OF THE HCN PRODUCTS

E. Carrasquillo-Molina and T. He, Department of Chemistry, University of Houston, Houston, TX 77204, Fax (713) 743-2709, e-mail: MCarrasquillo@uh.edu, the@bayou.uh.edu, and J. Adamson, Intellectual Property Services, OSP 4714, Shell Oil Co. (Presented at the *222nd National Meeting of the American Chemical Society*, Held in Chicago IL, August 2001).

Previous spectroscopic studies at high vibrational excitation utilized collisional relaxation to probe the ground and first excited electronic states of HCN. Those studies led to efficient LIF detection capabilities for vibrationally energized HCN molecules. This presentation will discuss the application of those capabilities to probe the $CN+C_2H_6$ and $CN+CH_4$ reactions by state resolution of the vibrationally energized HCN products. In these experiments, the HCN molecules produced were probed by LIF via the first excited electronic state. The temporal dependence of $HCN(v_1,v_2,v_3)$ was followed and state-specific bimolecular rate constants derived. These investigations succeeded in resolving initial vibrational state distributions, which provide for a detailed test of the reaction mechanism.

STATE-TO-STATE DIFFERENTIAL CROSS SECTIONS OF THE REACTION OF OVERTONE EXCITED METHANE WITH ATOMIC CHLORINE

Z.H. Kim, H.A. Bechtel and R.N. Zare, Department of Chemistry, Stanford University, Mudd Chemistry Building, Rothway M/C 5080, Stanford, CA 94305, Fax (650) 725-0259, e-mail: zhkim@leland.stanford.edu, hbechtel@leland.stanford.edu (Presented at the *222nd National Meeting of the American Chemical Society*, Held in Chicago IL, August 2001).

The reaction of $CH_4(\nu_3=2)$ with chlorine atoms is studied using the photoloc (photo-initiated reaction by law-of-cosines) technique. Measured state-to-state differential cross sections, integral cross sections, and speed-dependent spatial anisotropies of the HCl and CH_3 products indicate that a significant fraction of the CH_4 reagent vibrational energy is channeled into vibrational energy of the CH_3 product. These results are in stark contrast to the reaction of fundamentally excited $CH_4(\nu_3=1)$ with chlorine atoms, which shows no CH_3 vibrational excitation.

REACTION OF OVERTONE EXCITED METHANE WITH ATOMIC CHLORINE: STATE-TO-STATE DIFFERENTIAL CROSS SECTIONS AND VECTOR CORRELATIONS

Z.H. Kim, H.A. Bechtel and R.N. Zare, Department of Chemistry, Stanford University, Mudd Chemistry Building, Rothway M/C 5080, Stanford, CA 94305, Fax (650) 725-0259, e-mail: zhkim@leland.stanford.edu, hbechtel@leland.stanford.edu (Presented at the *222nd National Meeting of the American Chemical Society*, Held in Chicago IL, August 2001).

The reaction of $CH_4(\nu_3=2)$ with chlorine atoms is studied using the photoloc (photo-initiated reaction by law-of-cosines) technique. Measured state-to-state integral, differential cross sections, and the speed-dependent spatial anisotropies of HCl and CH_3 products show that a significant fraction of the CH_4 reagent vibrational energy is channeled into vibrational energy of the CH_3 product. The angular distributions of HCl product suggest the different mechanisms for each HCl(v=0,1, and 2) product channels. In order to gain further insight into reaction mechanisms, the effects of CH_4 reagent alignment on reactivity, and the product rotational polarizations are studied.

STATE-SELECTIVE PHOTODECOMPOSITION OF ClNO IN THE REGION 295-355 nm

D. Baugh, E. Torres and B. Alleyne, Department of Chemistry, UCLA, Los Angeles, CA 90095, e-mail: baugh@chem.ucla.edu (Presented at the *222nd National Meeting of the American Chemical Society*, Held in Chicago IL, August 2001).

The objective in state-to-state studies of fast photo-initiated unimolecular reactions is to determine structural and dynamical information regarding the molecular fragmentation process. The most fundamental of this information is the magnitude and phase of the transition amplitudes that connect the initial and final state wavefunctions, that is T-matrix elements. Indeed, selecting the states of the parent and resolving the states of the products provide the ultimate test for electronic structure computations as well as for quantal scattering methodology. Towards this end, studies of the 295-355 nm, state-selected photodecomposition of the atmospherically relevant, model triatomic ClNO will be reported. The UCLA hexapole was used to prepare molecular beams of ClNO in single rotational energy levels and with well defined laboratory velocities. Moreover, these molecules are not only energy level-selected but are magnetic (M) state polarized, that is orientated/aligned. M-state polarization of the energy level selected parent allows straightforward determination of the magnitudes and phases of the T-matrix elements, which were measured and are being reported for the photodecomposition of ClNO from 295 to 355 nm. The T-matrix elements were extracted from measurements of the differential and angle integrated alignment/orientation moments from the energy level specific detection of NO via (1+1) REMPI. Knowledge of the T-matrix elements' phases as a function of photolysis laser energy also appears to yield femtosecond scale time domain information regarding the reaction-using nanosecond lasers. The implications of which are obvious!

TIME-RESOLVED STUDIES OF THE VIBRATIONAL STATE POPULATIONS OF NO(X^2P,v=1-7) FOLLOWING NO_2 PHOTODISSOCIATION AT 193 nm USING FOURIER TRANSFORM INFRARED EMISSION SPECTROSCOPY

Y. Gong and B.R. Weiner, Department of Chemistry, University of Puerto Rico, Rio Piedras, San Juan, PR 00931, Fax (787) 756-7717, e-mail: gong@adam.uprr.pr, and X. Chen, University of Puerto Rico, Rio Piedras (Presented at the *222nd National Meeting of the American Chemical Society*, Held in Chicago IL, August 2001).

Vibrational state specific rate constants for the NO($X^2\Pi$, v=1-7) product resulting from NO_2 photodissociation at 193 nm have been measured by Time-Resolved Fourier Transform Infrared Emission Spectroscopy (TR-FTIRES). The nascent distribution of the vibrational state populations of NO($X^2\Pi$, v=1-7) is found to be non-Boltzmann. Rates for both the decay of the NO($X^2\Pi$, v=1-7) and the growth of $NO_2(\nu_3)$ have been simultaneously detected. The rotationally-resolved spectrum of the NO($X^2\Pi$,v) product has also been obtained by TR-FTIRES at 0.5 cm^{-1} spectral resolution.

RATE CONSTANTS AND KINETIC ISOTOPE EFFECT FOR THE FOUR-CENTERED ELIMINATION OF HF AND HCl FROM CHEMICALLY ACTIVATED $CF_3CFClCH_3$ AND $CF_3CFClCD_3$: A TEST OF THE 1,2-FCl REARRANGEMENT PATHWAY FOR HALOCARBONS

M.O Burgin and B.E. Holmes, Department of Chemistry, The University of North Carolina at Asheville, One University Heights, Asheville, NC 28804, Fax (828) 232-5179 (Presented at the *222nd National Meeting of the American Chemical Society*, Held in Chicago IL, August 2001).

We have previously observed $CF_3CF=CH_2$ and $CF_3CF=CD_2$ as a product in the unimolecular decomposition of chemically activated $CF_2ClCF_2CH_3$ and $CF_2ClCF_2CD_3$ respectively [*J. Phys. Chem.* A 2001, 105, 1615]. The reaction mechanism is formally a 1,3-HCl elimination with concurrent 1,2-F migration, but we proposed a two step mechanism consisting of a 1,2-FCl rearrangement forming $CF_3CFClCH_3$($CF_3CFClCD_3$) followed by a 2,3-HCl(2,3-DCl) elimination. The present results will test this novel mechanism by preparing chemically activated $CF_3CFClCH_3$($CF_3CFClCD_3$), with about 100 kcal/mol of internal energy. The unimolecular rate constants for the 4-centered elimination of hydrogen halides from $CF_3CFClCH_3$($CF_3CFClCD_3$) are: 4.1×10^6 s^{-1}(1.3×10^6 s^{-1}) for HCl loss and 5.1×10^5 s^{-1}(1.5×10^5 s^{-1}) for HF loss, the branching ratio is 7.9 (8.6). The isotope effect for 2,3-HCl/DCl is 3.2(±0.2) and the isotope effect for 2,3-HF/DF loss is 3.5(±0.2). These experimental rate constants and isotopes effects will be compared to data extracted from the $CF_2ClCF_2CH_3$ and $CF_2ClCF_2CD_3$ study to determine whether they are consistent with the two step mechanism: 1,2-FCl rearrangement/2,3-HCl elimination.

UNIMOLECULAR RATE CONSTANTS AND KINETIC ISOTOPE EFFECTS FOR DECOMPOSITION OF CHEMICALLY ACTIVATED $CF_2BrCF_2CH_3$ AND $CF_2BrCF_2CD_3$: EVIDENCE FOR A NOVEL 1,2-FBr INTERCHANGE

C.E. Lisowski, G.L. Heard and B.E. Holmes, Department of Chemistry, The University of North Carolina at Asheville, One University Heights, Asheville, NC 28804 (Presented at the *222nd National Meeting of the American Chemical Society*, Held in Chicago IL, August 2001).

Unimolecular rate constants and kinetic isotope effects have been measured for decomposition of $CF_2BrCF_2CH_3$ and $CF_2BrCF_2CD_3$ chemically activated with about 100 kcal/mol of internal energy. Two principal decomposition products for $CF_2BrCF_2CH_3$ were $CF_3CF=CH_2$, suggesting a 1,3-HBr elimination together with 1,2-F migration, and $CF_2BrCF=CH_2$, a 2,3-HF loss. The experimental rate constants for $CF_2BrCF_2CH_3$($CF_2BrCF_2CD_3$) were 1.4×10^5 s^{-1}(1.2×10^5 s^{-1}) for the 1,3-HBr process and 1.9×10^5 s^{-1}(0.63×10^5 s^{-1}) for the 2,3-HF elimination. The kinetic isotope effects were 1.2 for the 1,3-HBr elimination and 3.0 for the HF elimination process. Theoretical rate constants and kinetic isotope effects were calculated using RRKM theory and density functional theory to compute all the data necessary for the RRKM calculations. The agreement between the computed and experimental results suggests that the 1,3-HBr elimination is a two step mechanism consisting of a 1,2-FBr rearrangement forming $CF_3CFBrCH_3$, as the rate limiting step, and subsequent 2,3-HBr elimination to give the $CF_3CF=CH_2$.

1,2-FCl Rearrangement of CF_3CH_2Cl: An Alternative Pathway for CF_2CHF Production

P.T. Beaton, G. Heard and B.E. Holmes, Department of Chemistry, University of North Carolina at Asheville, One University Heights, Asheville, NC 28804, Fax (828) 232-5179 (Presented at the *222nd National Meeting of the American Chemical Society*, Held in Chicago IL, August 2001).

Ab initio and density functional theory calculations were performed for 1,1,1-trifluoro-2-chloroethane modeling several competing unimolecular reaction pathways including the 1,2-FCl interchange recently proposed by our group [*J. Phys. Chem.* A 2001, 105, 1615] for CF_3CH_2Cl. Computations at an energy of 97 kcal/mol using the B3PW91/6-311+G(2d,p) basis along with RRKM theory give threshold energy barriers, E_0, and unimolecular rate constants of 67.9 kcal/mol and $1.7 x 10^7$ s^{-1} for 1,2-FCl rearrangement of CF_3CH_2Cl to CF_2ClCH_2F, and 68.4 kcal/mol and $7.0 x 10^6$ s^{-1} for 1,2-HF elimination. The barriers for both 1,1-HCl elimination and C-Cl bond rupture of CF_3CH_2Cl are at least 10 kcal/mol higher. The 1,2-FCl rearrangement of CF_3CH_2Cl to CF_2ClCH_2F is endoergic by 11.3 kcal/mol. The calculations for CF_2ClCH_2F indicate E_0(1,2-HCl)=58.8 kcal/mol, E_0(1,2-HF)=67.0 kcal/mol producing the Z-isomer, and E_0(1,2-HF)=67.7 kcal/mol producing the E-isomer. Previously, the decomposition pathway for production of CF_2CHF following thermal, laser, or chemical activation of CF_3CH_2Cl has been assumed to be 1,1-HCl elimination forming the CF_3CH carbene which subsequently undergoes 1,2-F migration forming CF_2=CHF. The present results suggest an alternate pathway to CF_2=CHF from CF_3CH_2Cl: rearrangement to CF_2ClCH_2F followed by 1,2-HCl elimination. Analysis of all reaction pathways for both molecules will be presented along with comparisons to experimental kinetic data at least 10 kcal/mol higher. The 1,2-FCl rearrangement of CF_3CH_2Cl to CF_2ClCH_2F is endoergic by 11.3 kcal/mol. The calculations for CF_2ClCH_2F indicate E_0(1,2-HCl)=58.8 kcal/mol, E_0(1,2-HF)=67.0 kcal/mol producing the Z-isomer, and E_0(1,2-HF)=67.7 kcal/mol producing the E-isomer. Previously, the decomposition pathway for production of CF_2=CHF following thermal, laser, or chemical activation of CF_3CH_2Cl has been assumed to be 1,1-HCl elimination forming the CF_3CH carbene which subsequently undergoes 1,2-F migration forming CF_2=CHF. The present results suggest an alternate pathway to CF_2=CHF from CF_3CH_2Cl: rearrangement to CF_2ClCH_2F followed by 1,2-HCl elimination.

Alignment and Orientation in the $H+H_2O$ Reaction

G.C. Schatz, Department of Chemistry, Northwestern University, 2145 Sheridan Rd., Evanston, IL 60208, schatz@chem.nwu.edu, Diego Troya, University of La Rioja, and G. Lendvay, Hungarian Academy of Science (Presented at the *222nd National Meeting of the American Chemical Society*, Held in Chicago IL, August 2001).

We present the results of quasiclassical trajectory calculations of cross sections, product state distributions, angular distributions and OH alignment and orientation factors for the title reactions and isotopic counterparts involving deuterium. The calculations are based on a recently developed potential surface that was derived from high quality ab initio calculations. The calculations demonstrate an important correlation between product angular and alignment factors and product OH rotational state. These results are in very good agreement with recent measurements in Brouard's group. We also present results concerning measurements by Smith's group concerning the effect of local mode excitation on the branching between energy transfer and reaction in the title reaction.

Full Dimensional Quantum Study of Resonance Scattering for Reaction: Li+HF=H+LiF

L. Wei, Department of Chemistry, University of Minnesota, Minneapolis, MN 55455, e-mail: wei@t1.chem.umn.edu, and D.G. Truhlar, Department of Chemistry, University of Minnesota (Presented at the *222nd National Meeting of the American Chemical Society*, Held in Chicago IL, August 2001).

The accurate calculation of state-to-state, state-specific and cumulative reaction probabilities is presented for the bimolecular collision Li+HF=H+LiF in the total energy range from 0.26 to 0.50 eV on its ground electronic state potential energy surface. The calculated energy dependence of these reaction probabilities display a strong resonant structure. In contrast to the previous studies, we find

these long-lived resonances in both lower energy and higher energy ranges above threshold. We attribute this to the topology of the PES of the system. They are Feshbach resonances. These resonance states are identified by a combination of scattering and bound state calculations. Their lifetimes or the decay rates are obtained by fitting the calculated eigenphase sum to the Breit-Wigner formula. Their quantum numbers are assigned from the bound state calculations. The partial widths or branching ratios for the product states of these resonances are also calculated.

THE DIRECT CALCULATION OF DIABATIC STATES BASED ON CONFIGURATIONAL UNIFORMITY

H. Nakamura and D.G. Truhlar, Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455 (University of Minnesota Supercomputing Institute Research Report UMSI 2001/106, September 2001).

In order to provide a practical framework for the calculation of diabatic (technically quasidiabatic) states, we generalize the diabatization procedures of Atchity and Ruedenberg to include more general types of crossings and avoided crossings of potential energy surfaces. The resulting diabatization procedure involves two steps: (I) the construction of diabatic orbitals and (ii) the construction of many-electron diabatic state functions in terms of the diabatic orbitals. The procedure for step (I) is more general than the previously proposed occupation number and natural orbital method, and the procedure for step (ii) remains valid even for chemical reactions that require multiple diabatic prototypes. The method is illustrated by applications to LiH, ozone, H_2 dimer, and the reaction $Li(^2S,^2P) + HF \rightarrow LiF + H$.

KINETIC MEASUREMENTS OF THE QUENCHING OF CO_2(010) BY O ATOMS

K.J. Castle, E.S. Hwang and J.A. Dodd, VSBT, Air Force Research Laboratory, 29 Randolph Rd., Hanscom AFB, MA 01731, Fax (781) 377-8900, e-mail: karen.castle@hanscom.af.mil (Presented at the *222nd National Meeting of the American Chemical Society*, Held in Chicago IL, August 2001).

The goal of the present experiment is to directly measure the rate of relaxation of the ν_2 bending vibrational mode (010) of CO_2 by ground state oxygen atoms, $O(^3P)$. A principal source of cooling in the 70-120 km altitude region of the upper atmosphere occurs via collisional excitation of the CO_2 ν_2 mode, followed by 15 µm infrared emission into space. Collisions of ground vibrational state CO_2 with atomic oxygen are thought to be the most efficient means of populating the ν_2 state, but the vibrational energy transfer rate constant for the related relaxation process is not generally agreed upon. One possible means of determining the rate involves photolysis of NO_2 in a system containing CO_2. The photolysis simultaneously produces O atoms and induces a temperature jump of the system. The subsequent reequilibration of the (010) population at the new temperature is monitored with an infrared diode laser, resulting in a direct measure of the rate constant. Alternatively, a more sophisticated method of pumping the bend state of CO_2, stimulated Raman excitation, can be used.

COOPERATIVE MOLECULAR MODELING EXERCISE: THE HYPERSURFACE AS CLASSROOM

C.J. Cramer, B.L. Kormos, P. Winget, V.M. Audette, J.M. Beebe, C.S. Brauer, W.R. Burdick, E.W. Cochran, B.M. Eklov, T.J. Giese, Y. Jun, L.S.D. Kesavan, C.R. Kinsinger, M.E. Minyaev, R. Rajamani, J.S. Salsbury, J.M. Stubbs, J.T. Surek, J.D. Thompson, V.A. Voelz, C.D. Wick and L. Zhang, Department of Chemistry and Supercomputer Institute, University of Minnesota, 207 Pleasant St. SE, Minneapolis, MN 55455 (Published in *J. Chem. Ed.*, 2001).

A molecular modeling exercise and an associated exam that involve both competitive and cooperative learning aspects are described. Collaborative efforts are facilitated by web-based information management. The exercise/exam is appropriate for use in undergraduate or graduate quantum chemistry or molecular modeling courses that have access to modest computational resources. Students develop a molecular potential energy surface, identify multiple minima and transition state structures, repeat the process at two or more levels of theory, and then analyze the data looking for interesting chemical or computational phenomena.

TECHNICAL MEETINGS

(Current Additions to this List are Indicated by a Diamond Bullet Marking)

OCTOBER 1-4, 2001

EASTERN ANALYTICAL SYMPOSIUM
Atlantic City NJ.

> Information: Eastern Analytical Symposium and Exposition Inc., P.O. Box 633, Montchanin, DE 19710, (302) 738-6218, Fax (302) 738-5275, e-mail: easinfo@aol.com, http://www.eas.org

OCTOBER 1-5, 2001

6th INTERNATIONAL CONFERENCE ON LASER ABLATION
Tsukuba, Japan.

> Information: K. Murakami, COLA'01 Office, Institute of Applied Physics, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan (81) 298-53-5272, Fax (81) 298-55-7440, e-mail: murakami@ims.tsukuba.ac.jp, http://cola.ims.tsukuba.ac.jp/

OCTOBER 4-6, 2001

AMERICAN PHYSICAL SOCIETY TEXAS SECTION FALL MEETING
Fort Worth TX.

> Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 5-6, 2001
34th MIDWEST THEORETICAL CHEMISTRY CONFERENCE
Minneapolis MN.

> Information: M. Olesen, Conference Adminstrator, Minnesota Supercomputing Institute, University of Minnesota, 1200 Washington Avenue South, Minneapolis, MN 55415, (612) 624-1356, Fax (612) 624-8861, e-mail: mtcc@msi.umn.edu, http://www.msi.umn.edu/general/ Symposia/MTCC/index2.html

OCTOBER 5-12, 2001

28th ANNUAL MEETING OF THE FEDERATION OF ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES
Detroit MI.

> Information: C. Lilly, Federation of Analytical Chemistry and Spectroscopy Societies, 1201 Don Diego Ave., Santa Fe, NM 87505, (505) 820-1648, Fax (505) 989-1073, e-mail: jsjoberg@trail.com, http://facss.org/info.html

OCTOBER 9-11, 2001

INTERNATIONAL SYMPOSIUM ON COMBUSTION AND PLASMO-CHEMISTRY
Almaty, Kazakhstan.

Topics will Include:

- Theory of Combustion. Structure of Flame
- Kinetics and Mechanism of Chemical Reactions
- Turbulence. Turbulent Combustion
- Modeling of Chemical Processes
- Modeling of Plasmo-Chemical Processes and Fuel Use
- Plasmo-Chemistry of Surface Coating and Strengthening
- Plasma Metal Cutting and Natural and Construction Material Processing
- Plasma Technologies of Fuel Ignition, Combustion and Gasification
- Soot and Fullerene Formation in the Processes of Combustion
- Technological Combustion
- Self-propagating High-Temperature Synthesis
- Thermal Processes in Oil and Gas Processing

Information: Z.A. Mansurov, Combustion Problems Institute, Bogenbay Batyr Str., 172, Almaty, Kazakhstan 480012, (3272) 92-43-46, Fax (3272) 92-58-11, e-mail: icp@nursat.kz; mansurov@lorton.com, http://eurasianchemtech.vub.ac.be/
Deadline:Abstracts to be Submitted by September 1, 2001.

OCTOBER 9-12, 2001
54th ANNUAL GASEOUS ELECTRONICS CONFERENCE
University Park PA.

Information: R.T. McGrath, (814) 863-9580, Fax (814) 863-9659, e-mail: mcgrath@psu.edu, http://www.engr.psu.edu/cde/GEC54.html

OCTOBER 10-13, 2001

36th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Lincoln NE.

Information: D. Berkowitz, Department of Chemistry, University of Nebraska, Lincoln, NE 68588-0304, (402) 472-2738, Fax (402) 472-9402, e-mail: dbb@unlinfo.edu

OCTOBER 14-18, 2001

6th INTERNATIONAL SYMPOSIUM ON SELF PROPAGATING HIGH TEMPERATURE SYNTHESIS
Haifa, Israel.

Information: I. Gotman, Technion-Israel Institute of Technology, Department of Materials Engineering, Technion, Haifa, Israel 32000, (972) 4-829-2112, Fax (972) 4-832-1978, e-mail: gotman@techunix.technion.ac.il, http://www.technion.ac.il/technion/materials/conferences.html

OCTOBER 14-19, 2001

INTERNATIONAL SYMPOSIUM ON VISUALIZATION AND IMAGING IN TRANSPORT
Antalya, Turkey.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-1429, Fax (90) 312-210-1331, arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

OCTOBER 14-19, 2001

OPTICAL SOCIETY OF AMERICA 2001 ANNUAL MEETING AND THE 17TH INTERDISCIPLINARY LASER SCIENCE CONFERENCE
Long Beach CA.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, Fax (202) 416-6100, e-mail: confserv@osa.org, http://www.osa.org/mtg_conf

OCTOBER 15-16, 2001

WESTERN STATES SECTION MEETING OF THE COMBUSTION INSTITUTE
Salt Lake City UT.

Information: W.J. Pitz, Secretary, Western States Section of the Combustion Institute, Lawrence Livermore National Laboratory, L-091, P.O. Box 808, Livermore, CA 94551, (925) 422-7730, Fax (925) 423-8772, e-mail: pitz@llnl.gov, http://www.wssci.org/

OCTOBER 15-18, 2001

ICALEO '2001
Jacksonville, FL.

Topics Include:

- Laser Materials Processing Conference
- Laser Microfabrication Conference
- Plenary Session: Lasers and Nanotechnology
- Laser Solutions Technical Short Courses

Information: ICALEO, 13501 Ingenuity Drive, Suite 128, Orlando, FL 32826, (407) 380.1553, Fax (407) 380.5588, http://www.laserinstitute.org, or www.icaleo.org

OCTOBER 16-17, 2001

AIR POLLUTION CONFERENCE: ANNUAL SYMPOSIUM OF THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS, ENVIRONMENTAL ENGINEERING DIVISION, HONORING THE MEMORY OF DIXIE LEE RAY
Washington DC.

Topics will Include:

- Emerging Regulations
- Particulate Matter
- Advanced Pollution Control Technology
- Industry-Specific Issues

- Climate Change
- Air Toxics
- Continuous Emissions Monitoring

Information: S.G. Buckley, Department of Mechanical Engineering, 2181 Glenn L. Martin Hall, University of Maryland, College Park, MD 20742, (301) 405-8441, Fax (301) 314-9477, e-mail: buckley@eng.umd.edu

OCTOBER 16-19, 2001

57th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Antonio TX.

Information: S.T. Weintraub, Department of Biochemistry, University of Texas Health Science Center, 7703 Floyd Curl Drive, San Antonio, TX 78284, (210) 567-4043, Fax (210) 567-5524, e-mail: weintraub@uthscsa.edu

OCTOBER 19-20, 2001

OHIO SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Columbus OH.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 21-25, 2001

18th WORLD ENERGY CONGRESS
Buenos Aires, Argentina.

Information: World Energy Council, Del Carmen 766-4° Piso, 1019 Buenos Aires, Argentina, (54) 11-4-813-2219, Fax (54) 11-4-814-3664.

OCTOBER 23-26, 2001

36th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Ventura CA.

Information: R.W. Hurst, 9 Faculty Court, Thousand Oaks, CA 91360, (805) 492-7764, Fax (805) 241-7149, e-mail: Alarwh@aol.com

OCTOBER 26-27, 2001

OHIO SECTIONAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Granville OH.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 28-31, 2001

37th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Santa Barbara CA.

Information: R.W. Hurst, Hurst & Associates, 9 Faculty Court, Thousand Oaks, CA 91360, fax/phone (805) 492-7764, e-mail: alasrwh@aol.com

OCTOBER 28-31, 2001

PHOTONICS BOSTON
Newton MA.

Includes Symposia and Conferences on:
- Environmental and Industrial Sensing

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

OCTOBER 28-NOVEMBER 2, 2001

POWER PRODUCTION IN THE 21ST CENTURY: IMPACTS OF FUEL QUALITY AND OPERATIONS
Snowbird UT.

Topics will include:
- Physical Properties of Ash/Deposits
- Deposit Formation
- Deposit Removal
- Deposition Modeling
- Corrosion: Fundamental Studies
- Corrosion: Commercial Experience
- Soot Formation and Control
- Issues for Alternate Fuel Blends
- Diagnostics, Sensors, and Controls

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, http://www.engfnd.org/engfnd/conf.html

NOVEMBER 1-3, 2001

10th INTERNATIONAL CONFERENCE ON CURRENT TRENDS IN COMPUTATIONAL CHEMISTRY
Jackson MS.

Information: Miss J. Leszczynski, Jackson State University, Department of Chemistry, 1400 J.R. Lynch Street, Jackson, MS 39217, (601) 979-3482, Fax (601) 979-7823.

NOVEMBER 2-3, 2001

AMERICAN PHYSICAL SOCIETY FOUR CORNERS SECTION
Las Cruces NM.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 2-3, 2001

JOINT NEW ENGLAND SECTIONS FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY AND THE AMERICAN ASSOCIATION OF PHYSICS TEACHERS
Keene State College NH.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 2-3, 2001

9th INTERNATIONAL SYMPOSIUM ON LASER SPECTROSCOPY
Taejon, Korea.

Information: J. Lee, Korea Atomic Energy Research Institute, Laboratory for Quantum Optics, P.O. Box 105, Taejon 305-600, Korea, (82) 42-868-2135, Fax (82) 42-861-8292, e-mail: jmlee@kaeri.re.kr

NOVEMBER 4-6, 2001

AMERICAN PHYSICAL SOCIETY SOUTHEASTERN SECTION
Charlottesville VA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 4-9, 2001

ANNUAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Reno NV.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 3 Park Ave., 18th Floor, New York, NY 10016, (212) 591-7950, Fax (212) 591-8893, http://www.aiche.org

NOVEMBER 5-8, 2001

2001 INTERNATIONAL GAS RESEARCH CONFERENCE
Amsterdam, The Netherlands.

Information: D. Dolenc, (773) 399-8226, Fax (773) 399-4605, e-mail: igrc@gri.org, http://www.gri.org/IGRC2001

NOVEMBER 11-16, 2001

INTERNATIONAL ASME MECHANICAL ENGINEERING CONGRESS AND EXPOSITION
New York NY.

Sessions on
- Pool Fire Measurements and Simulations
- Open Forum on Fire and Combustion

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

NOVEMBER 18-20, 2001

DIVISION OF FLUID DYNAMICS MEETING OF THE AMERICAN PHYSICAL SOCIETY
San Diego CA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 26-30, 2001

FALL MEETING OF THE MATERIALS RESEARCH SOCIETY
Boston MA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, e-mail: info@mrs.org

NOVEMBER 28-30, 2001

2001 SAE SMALL ENGINE TECHNOLOGY CONFERENCE AND EXPOSITION
Pisa, Italy.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org
Submit your abstract of up to 500 words by November 2, 2000 to Karin Bolcshazy, SAE International, 400 Commonwealth Drive, Warrendale, PA 15096, (724) 772-7179, Fax (724) 776-1830, e-mail: karinb@sae.org
The abstract should include a tentative paper title, authors and co-authors (full names, position, company address, email, telephone and fax numbers).

DECEMBER 3-6, 2001

5th ASIA-OCEANIA SYMPOSIUM ON FIRE SCIENCE AND TECHNOLOGY
Callaghan, NSW, Australia.

Information: B.Z. Dlugogorski, Department of Chemical Engineering, The University of Newcastle, Callaghan, NSW 2308 Australia, 61-2-4921-6176, Fax 61-2-4921-6920, e-mail: cgbzd@alinga.newcastle.edu.au
Deadline: Submission of Full Papers by March 1, 2001.

DECEMBER 3-7, 2001

18th INTERNATIONAL PITTSBURGH COAL CONFERENCE, COAL'S INTERNATIONAL FUTURE: THE TECHNICAL CHALLENGE
Newcastle, New South Wales, Australia.

Information: Conference Secretary, Pittsburgh Coal Conference, University of Pittsburgh, 1130 Benedum Hall, Pittsburgh, PA 15261, (412) 624-7440, Fax (412) 624-1480, e-mail: pcc@engrng.pitt.edu, http://www.engrng.pitt.edu/~pccwww/

DECEMBER 9-14, 2001

14th AUSTRALASIAN FLUID MECHANICS CONFERENCE
Adelaide, Australia.

Information: 14th Australasian Fluid Mechanics Conference, Department of Mechanical Engineering, The University of Adelaide, SA 5005, Australia, (61) 8-8303 5397, Fax (61) 8-8303 4367, e-mail: afmc@mecheng.adelaide.edu.au, http://www.mecheng, adelaide.edu.au/14afmc/14afmc.htm

JANUARY 3-5, 2002

5th ISHMT/ASME HEAT AND MASS TRANSFER CONFERENCE
Calcutta, India.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7072, Fax (212) 705-7143, http://www.asme.org

JANUARY 6-11, 2002

2nd MEDITERRANEAN COMBUSTION SYMPOSIUM
Sharm El-Shaikh, Egypt.

Topics will Include:

- Turbulent Combustion and Modeling
- Flame Structure and Dynamics
- Sprays and Gas Combustion Systems
- Internal Combustion Engines
- Solid Fuels Combustion
- Optical Diagnostics and Radiative Transfer
- Fire/Explosions
- Combustion and Pollutants
- Kinetics

Information: M.S. Mansour, Department of Mechanical Engineering, The American University in Cairo, Cairo, Egypt, Fax (202) 795-7565, e-mail: mansourm@aucegypt.edu

JANUARY 6-12, 2002

WINTER CONFERENCE ON PLASMA SPECTROCHEMISTRY
Scottsdale AZ.

Information: R.M. Barnes, ICP Information Newsletter Inc., P.O. Box 666, Hadley, MA 01035, (413) 256-8942, Fax (413) 256-3746, e-mail: winterconf@chem.umass.edu, http://www.chem.umass.edu/WinterConf2002

JANUARY 21-23, 2002

3rd INTERNATIONAL SYMPOSIUM ON NON-CO_2 GREENHOUSE GASES
Maastricht, The Netherlands

Information: C. Hoefsloot, VVM Bureau, Baden Powellstraat 1/kamer 4.17, Postbus 2195, 's-Hertogenbosch, Netherlands 5212 BW, (011) 736215985, Fax (011) 736216985, e-mail: vvm@wxs.nl, http://www.milieukundigen.nl/ncgg-3.htm

♦ FEBRUARY 7-8, 2002

2002 AUSTRALIAN SYMPOSIUM ON COMBUSTION AND THE 7th AUSTRALIAN FLAME DAYS

Biennial Joint Meeting of the Australian/New Zealand Sections of the Combustion Institute and the Australian Flame Research Committee.
Information: http://www.ifrf.net/ifrf_net/meetings.html

FEBRUARY 7-10, 2002

LASERS TO CHEMICAL AND ENVIRONMENTAL ANALYSIS TOPICAL MEETING OF THE OPTICAL SOCIETY OF AMERICA
Boulder CO.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org, http://www.osa.org/mtg_conf

FEBRUARY 12-13, 2002

CUTTING NO_x: FORUM 2002
Houston TX.

Information: J.C. Smith, Institute of Clean Air Companies, 1660 L Street NW, Suite 1100, Washington DC, 20036, (202) 457-0911, Fax (202) 331-1388, e-mail: jsmith@icac.com

MARCH 4-7, 2002

SAE WORLD CONGRESS
Detroit MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

♦ MARCH 7-9, 2002

TEXAS SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY
Nacogdoches TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ MARCH 11-15, 2002

14th INTERNATIONAL COAL PREPARATION CONGRESS AND EXHIBITION
Johannesburg, South Africa.

Information: Conference Services, National Energy Technology Laboratory, U.S. Department of Energy, Morgantown WV, (412) 386-6044, Fax (412) 386-6486, e-mail: kimberly.yavorsky@netl.doe.gov

MARCH 18-22, 2002

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Indianapolis IN.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 18-22, 2002

PITTCON 2000: THE PITTSBURGH CONFERENCE
New Orleans LA.

Information: The Pittsburgh Conference, 300 Penn Center Blvd., Suite 332, Pittsburgh, PA 15235, (412) 825-3220, Fax (412) 825-3224, e-mail: pittconinfo@pittcon.org, http://www.pitcon.org/

♦ MARCH 25-26, 2002

SPRING MEETING OF THE WESTERN STATES SECTION OF THE COMBUSTION INSTITUTE
San Diego CA.

Information: W.J. Pitz, L-91, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551, (925) 422-7730, Fax (925) 423-8772, e-mail: pitz@llnl.gov, http://www.wssci.org

♦ APRIL 2-5, 2002

6th EUROPEAN CONFERENCE ON INDUSTRIAL FURNACES AND BOILERS
Lisbon, Portugal.

Information: A. Reis, Rua Gago Coutinho 185-187, 4435-034 Rio Tinto, Portugal, (351) 2297 34624, Fax (351) 2297 30746, e-mail: conference@infub.pt, http://www.infub.pt

APRIL 1-5, 2002

MATERIALS RESEARCH SOCIETY SPRING MEETING
San Francisco CA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, e-mail: info@mrs.org, http://www.mrs.org/meetings

APRIL 1-6, 2002

26th CONFERENCE ON STATIONARY SOURCE SAMPLING AND ANALYSIS FOR AIR POLLUTANTS
Destin FL.

Topics will Include:

- New Technologies
- EPA Test Method Development and Regulatory Update
- Data Quality
- Accreditation Status NELAC, EDIC, ASTM and SES Efforts.
- Safety
- International Testing Developments
- The Truth About Stack Sampling
- State Programs for Accreditation and Test Oversight Enforcement
- New Emission Testing Techniques

Information: B. Mullins, METCO Environmental Inc., P.O. Box 598, Addison, TX 75001, (972) 931-7127, Fax (972) 931-8398, e-mail: bmullins@testamericainc.com, or United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, http://www.engfnd.org/engfnd/conf.html

♦ APRIL 5-6, 2002

NEW ENGLAND SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY
Waltham MA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ APRIL 7-9, 2002

CENTRAL STATES SECTION SPRING MEETING OF THE COMBUSTION INSTITUTE
Knoxville TN.

Information: D.L. Reuss, General Motors R&D, (810) 986-0887, e-mail: dreuss@gmr.com, http://www.cssci.org

APRIL 7-10, 2002

9th International Conference on Numerical Combustion: Joint Meeting of Siam and the Italian Section of the Combustion Institute
Sorrento, Italy.

Topics will Include:

- Adaptive Numerical Methods
- Applications of Parallel Processing
- Detonation
- Droplets and Sprays
- Energetic Materials (Propellants and Explosives)
- Engine and Furnace Combustion
- Fires
- Flames
- Heterogeneous Combustion
- Ignition
- Kinetics
- Material Synthesis
- Microgravity
- Pollution
- Software Engineering for Combustion Applications
- Tera-Scale Computation of Combustion Applications
- Turbulence

Information: e-mail: icnc2002@unisannio.it, http://www.ing.unisannio.it/icnc2002
Deadlines: October 31, 2001 for Submission of Minisymposium Proposals, and November 30, 2001 for Submission of Contributed Abstracts.

♦ APRIL 7-12, 2002

223rd National Meeting of the American Chemical Society
Orlando FL.

Division of Fuel Chemistry:

- CO_2 Capture and Sequestration
- Hydrogen Production and Utilization
- Production and Utilization of Renewable Fuels
- Trends in Carbon Products
- Utilization of Greenhouse Gases

Information: R.P. Warzinski, Federal Energy Technology Center, U.S. Department of Energy, P.O. Box 10940, Pittsburgh, PA 15236, (412) 386-5863, Fax (412) 386-4152, e-mail: warzinski@fetc.doe.gov, or Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

Division of Physical Chemistry:

- Reaction Mechanisms: Kinetics and Catalysis, J. Golab, golabjt@bp.com; T. Truong, truong@chemistry.chem.utah.edu
- Chemistry and the Environment in the 21st Century: Environmental Chemistry at Interfaces, W. Flynn, flynn@chem.columbia.edu; P. Stair, pstair@northwestern.edu; E. Stiefel, eistief@erenj.com

- Frontiers in Chemical Dynamics, P. Houston, plh2@cornell.edu; H.F. Davis, hfd1@cornell.edu

Information: J.C. Hemminger, Department of Chemistry, University of California, Irvine, CA 92697, (949) 824-6020, Fax (949) 824-3168, jchemmin@uci.edu

♦ APRIL 12-13, 2002

OHIO SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY
Youngstown OH.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ APRIL 12-13, 2002

NEW YORK SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY
Oneonta NY.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

APRIL 14-17, 2002

ASME/INTERNAL COMBUSTION ENGINE DIVISION SPRING TECHNICAL CONFERENCE
Rockford IL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

APRIL 20-23, 2002

APRIL NATIONAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Albuquerque NM.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

APRIL 23-26, 2002

ANALYTICA 2002
Munich, Germany.

Information: Analytica, Messe Muchen GmbH, 81823 Muchen, Germany, (49) 89-9492-0380, Fax (49) 89-9492-0389, http://www.analytica.de

APRIL 29-MAY 1, 2002

5th INTERNATIONAL WORKSHOP ON CATALYTIC COMBUSTION
Seoul, Korea.

Topics will Include:

- Kinetics and Transport Processes in Catalytic Combustion
- Development of High Temperature Materials for Catalytic Combustion

- Application of Catalytic Combustion in Industrial Commercial and Residential Burners
- Commercialization of Low Emission Gas Turbine Catalytic Combustor

Information: Sung June Cho, Secretary, 5 IWCC, Korea Institute of Energy Research, 71-2, Jang-dong, Yusung-gu, Taejon 305-343, Korea, (82) 42-860-3613, Fax (82) 42-860-3133, e-mail: sjcho@kier.re.kr
Deadline: Submit Extended Abstract by July 31, 2001.

♦ APRIL 29-MAY 3, 2002

12th ANNUAL HALON OPTIONS TECHNICAL WORKING CONFERENCE
Albuquerque NM.

Information: R.G. Gann, Mail Stop 8664, NIST, 100 Bureau Drive, Gaithersburg, MD 20899, e-mail: rggann@nist.gov, http://www.bfrl.nist.gov/866/NGP

MAY 5-8, 2002

7th CIRCULATING FLUIDIZED BED CONFERENCE
Niagara Falls, Canada.

Information: AICUL Consulting, e-mail: aicul-con@home.com

MAY 12-17, 2002

201st MEETING OF THE ELECTROCHEMICAL SOCIETY
Philadelphia PA.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/199/meet.html

♦ MAY 17-18, 2002

NORTHWEST SECTIONAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Edmonton, Alberta, Canada.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ MAY 19-24, 2002

CONFERENCE ON LASERS AND ELECTROOPTICS (CLEO) AND ON QUANTUM ELECTRONICS AND LASER SCIENCE (QELS)
Long Beach CA.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 416-1907, Fax (202) 416-6100, e-mail: cust.serv@osa.org, http://www.osa.org/CLEO

♦ MAY 28-30, 2002

35th MIDDLE ATLANTIC REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Fairvax VA.

Information: G. Mushrush, George Mason University, Chemistry Department 3E2, 4400 University Drive, Fairfax, VA 22030, (703) 993-1070, Fax (703) 993-1389, e-mail: Gmushrus@gmu.edu

♦ JUNE 2-4, 2002

33rd GREAT LAKES REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Minneapolis, MN.

Information: N.W. Gladfelter, University of Minnesota, Department of Chemistry, 207 Pleasant Street, S.E., Minneapolis, MN 55455, (612) 624-6000, Fax (612) 626-8659, e-mail: gladfelt@chem.umn.edu

JUNE 2-6, 2002

6th INTERNATIONAL CONFERENCE ON CHEMICAL STRUCTURES
Noordwijkerhout, The Netherlands.

Information: G. Grethe, MDL Information Systems, 14600 Catalina Street, San Leandro, CA 94577, (510) 357-2222 ext. 1430, Fax (510) 614-3616, e-mail: guenter@mdli.com, http://www.lib.uchicago.edu/cinf/cinf_meetings.html

JUNE 2-6, 2002

50th ASMS CONFERENCE ON MASS SPECTROMETRY
Orlando FL.

Information: American Society for Mass Spectrometry, 1201 Don Diego Avenue, Santa Fe, NM 87505, (505) 989-4517, Fax (505) 989-1073, e-mail: asms@asms.org

JUNE 3-6, 2002

ASME TURBO EXPO: LAND, SEA AND AIR
Amsterdam, The Netherlands.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (404) 847-0072, Fax (212) 705-7143, http://www.asme.org

JUNE 4-7, 2002

10th INTERNATIONAL SYMPOSIUM ON ANALYTICAL CHEMISTRY
Granada, Spain.

Information: Dr. A.M. Garcia-Campana, Department Analytical Chemistry, Faculty Sciences, University of Granada, Av. Fuentenueva s/n, Granada, Spain, 34 (9) 58-24-85-94; Fax 34 (9) 58-24-33-288, e-mail: amgarcia@goliat.ugr.es

JUNE 9-13, 2002

4th Oxford Conference on Spectrometry
Davidson NC.

Information: A. Springsteen, Avian Technologies, P.O. Box 1076, New London, NH 03257, (603) 525-4479, Fax (603) 526-4087, e-mail: arts@aviantechnologies.com

JUNE 10-13, 2002

ASME Summer Annual Meeting
Minneapolis MN.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7795, Fax (212) 705-7143, http://www.asme.org

♦ JUNE 19-21, 2002

57th Northwest Regional Meeting of the American Chemical Society
Spokane WA.

Information: D. DeMattia, North 4906 Northwood Dr., Spokane, WA 99212, (509) 926-6011, Fax (509) 926-6130 e-mail: dennis@byte-dynamics.com

JUNE 20-22, 2002

57th Northwest Regional Meeting of the American Chemical Society

Information: D. Cleary, Chemistry Department, Gonzaga University, Spokane, WA 99258, (509) 323-6631, e-mail: cleary@gonzaga.edu

JUNE 23-27, 2002

Air and Waste Management Association Annual Conference
Baltimore MD.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

JUNE 22-28, 2002

International quantum Electronics Conference and the Conference on Lasers, Applications and Technologies
Moscow, Russia.

Information: M.V. Lomonosov Moscow State University, 7(095) 939-51-73, Fax 7(095) 939-31-13, e-mail: iquec2002@comsim1.phys.msu.su, http://www.ilc.msu.su/iqec2002/

JUNE 23-28, 2002

14th US NATIONAL CONGRESS OF APPLIED MECHANICS
Blacksburg VA.

Information: W. Hylton, Continuing Education, Mail Code 0364, Virginia Tech, Blacksburg, VA 24060, (540) 231-9617, Fax (540) 231-9886, e-mail: whylton@vt.edu
Deadline: Submission of Abstract by January 31, 2002.

JUNE 24-26, 2002

TIME RESOLVED CHEMISTRY: FROM STRUCTURE TO FUNCTION. GENERAL DISCUSSION NUMBER 122 OF THE FARADAY DIVISION OF THE ROYAL SOCIETY OF CHEMISTRY
Manchester UK.

Topics will Include:

- Technique Developments for Time-Resolved and Dynamical Studies
- Enzyme Structural Intermediates and Catalytic Action
- Computer Modeling of Chemical Processes
- Signal Transduction and Photo-Induced Structural Changes
- Chemical Structural Intermediates and Catalysis
- Materials and Polymer Processing

Information: http://www.rsc.org/lap/confs/faradischome.htm

♦ JUNE 26-29, 2002

34th CENTRAL REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Ypsilanti MI.

Information: D. Snyder, Eastern Michigan University, 215 Mark Jefferson Science Center, Ypsilanti, MI 48197, (734) 487-1429, Fax (734) 487-1496, e-mail: donald.snyder@emich.edu

JULY 7-10, 2002

4th INTERNATIONAL SYMPOSIUM ON COAL STRUCTURE
Gliwice, Poland.

Topics will Include:

- Physical and Chemical Structure of Coal and Carbonaceous Materials
- Reactivity and Modifications of Coal and Carbonaceous Materials
- Carbonization and Graphitization
- Fibers and Advanced Carbonaceous Materials
- Novel Forms of Carbon
- Porous Carbonaceous Materials (Adorbents, Catalytic Supports, etc.)
- Technical Applications

Information: J. Pajak, Institute of Coal Chemistry, Polish Academy of Sciences, 48(32) 2380770, Fax 48(32) 2312831, e-mail: cs2002@karboch.gliwice.pl, http://www.karboch.gliwice.pl/cs2002
Deadline: For Abstracts: April 30, 2001, for papers: January 31, 2002. The accepted papers will be published in a special issue of *Fuel Processing Technology*. Only short papers or extended abstracts up to 5 pages will be accepted.

JULY 14-19, 2002

19th IUPAC SYMPOSIUM ON PHOTOCHEMISTRY

Budapest, Hungary.

Topics Emphasize Biological and Organic Chemistry.

Information: H.D. Roth, Department of Chemistry and Chemical Biology, Rutgers University, 610 Taylor Road, New Brunswick, NJ 08854, (732) 445-5664, Fax (732) 445-5312, e-mail: roth@rutchem.rutgers.edu, http://www.photoiupac.hu

JULY 21-26, 2002

29th INTERNATIONAL SYMPOSIUM ON COMBUSTION

Sapporo, Japan.

Information: S. Terpack, The Combustion Institute, 5001 Baum Boulevard, Suite 635, Pittsburgh PA 15213, (412) 687-1366, Fax (412) 687-0340, e-mail: office@combustioninstitute.org

JULY 21-26, 2002

4th WORLD CONGRESS ON PARTICLE TECHNOLOGY

Sydney, Australia.

Information: J. Hatte, Conference Coordinator, ICMS Australasia Pty Ltd., Level 6, 2 Bridge Street, Sydney NSW 2000, (61) 2-9241-1478, Fax (61) 2-9251-3552, e-mail: josie@icmsaust.com.au, http://www.wcpt4.com/

JULY 28-AUGUST 2, 2002

17th IUPAC CONFERENCE ON CHEMICAL THERMODYNAMICS

Information: A. Heintz, Universitat Rostock, FB Chemie, Hermannstr. 14, 180512 Rostock, Germany, (49) 381-498-1852, Fax (49) 381-498-1854, e-mail: andreas.heintz@chemie.uni-rostock.de, http://www.iupac.org/symposia/

AUGUST 4-9, 2002

14th INTERNATIONAL CONFERENCE ON PHOTOCHEMICAL CONVERSION AND STORAGE OF SOLAR ENERGY

Sapporo, Japan.

Topics will Include:

- Photoinduced Electron Transfer Processes
- Photochemical Conversion
- Photoelectrochemistry
- Photocatalysis
- Photosynthesis
- Time Resolved and Coherent Spectroscopy

Information: The Secretariat IPS-14: EC Inc., President Building 5F, Minami-1, Nishi-5, Chuo-ku, Sapporo, 060-0061, Japan, (81) 11-231-2289, Fax (81) 11-221-0496, e-mail: ips14@ec-inc.co.jp, http://www.ec-inc.co.jp/ips14

AUGUST 18-22, 2002

224th National Meeting of the American Chemical Society
Boston MA.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

♦ SEPTEMBER 1-5, 2002

17th World Petroleum Congress
Rio de Janeiro, Brazil.

Information: http://www.world-petroleum.org

SEPTEMBER 8-13, 2002

6th International Aerosol Conference
Taipei, Taiwan.

Information: CAART, C.-J. Tsai, Institute of Environmental Engineering, National Chiao Tung University, Hsin Chu, Taiwan, (886) 3-5731880, Fax (886) 3-57727835, e-mail: cjtsai@green.ev.nctu.edu.tw, http://jeff.che.nthu.edu.tw.caart/

♦ SEPTEMBER 17-20, 2002

5th International Symposium on Gas Cleaning at High Temperature
Morgantown WV.

Information: Conference Services, National Energy Technology Laboratory, U.S. Department of Energy, Morgantown WV, (412) 386-6044, Fax (412) 386-6486, e-mail: kimberly.yavorsky@netl.doe.gov, http://www.netl.doe.gov

♦ SEPTEMBER 29-OCTOBER 2, 2002

Laser Science XVIII
Orlando FL.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ OCTOBER 4-5, 2002

Four Corners Section Meeting of the American Physical Society
Salt Lake City UT.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 6, 2002

202nd MEETING OF THE ELECTROCHEMICAL SOCIETY
Salt Lake City UT.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/199/meet.html

♦ OCTOBER 10-12, 2002

TEXAS SECTIONAL FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Brownsville TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ OCTOBER 11-12, 2002

NEW YORK SECTIONAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Syracuse NY.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ OCTOBER 12-14, 2002

17th ROCKY MOUNTAIN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Albuquerque NM.

Information: D. Porterfield, Los Alamos National Laboratory, P.O. Box 1663, NMT-1, Los Alamos, NM 87545, (505) 667-4710, Fax (240) 358-1192, e-mail: dporterfield@lanl.gov

♦ OCTOBER 15-18, 2002

55th GASEOUS ELECTRONICS CONFERENCE
Minneapolis MN.

Information: e-mail: gec@me.umn.edu, http://www.me.umn.edu/gec/

♦ OCTOBER 18-19, 2002

OHIO SECTIONAL FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Columbus OH.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 21-24, 2002

8th Symposium on Temperature: Its Measurement and Control in Science and Industry
Chicago IL.

Information: D.N. Dunkley, 8th Symposium on Temperature, ISA, P.O. Box 12277, 67 Alexander Drive, Research Triangle, NC 12277, e-mail: ddunkley@isa.org

♦ OCTOBER 23-25, 2002

37th Midwest Regional Meeting of the American Chemical Society
Lawrence KS.

Information: R. Carlson, University of Kansas, Department of Chemistry, Malott Hall, Lawrence, KS 66045-0001, (785) 864-3686, Fax (785) 864-5396, e-mail: rcarlson@ukans.edu

OCTOBER 23-26, 2002

38th Western Regional Meeting of the American Chemical Society
San Francisco CA.

Information: N.D. Byington, U.S. Customs Service Laboratory, 630 Sansome St., Room 1407, San Francisco, CA 94111, (415) 705-4405 ext. 216, Fax (415) 705-4236, e-mail: neal@byington.org

♦ OCTOBER 30-NOVEMBER 2, 2002

Southeast Sectional Meeting of the American Physical Society
Auburn AL.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ NOVEMBER 3-6, 2002

58th Southwest Regional Meeting of the American Chemical Society
Austin TX.

Information: P. Barbara, University of Texas, Department of Chemistry and Biochemistry, Welch Hall, Austin, TX 78712, (512) 471-2880, Fax (512) 471-8696, e-mail: pbarbara@mail.utexas.edu

♦ NOVEMBER 13-17, 2002

54th Southeast Regional Meeting of the American Chemical Society
Charleston SC.

Information: G.P. Meier, Department of Pharmaceutical Sciences, Medical University of South Carolina, 280 Calhoun St., P.O. Box 250140, Charleston, SC 29425, (843) 792-8445, Fax (843) 792-0759, e-mail: meiergp@musc.edu

NOVEMBER 17-22, 2002

INTERNATIONAL MECHANICAL ENGINEERING CONGRESS AND EXPOSITION, THE WINTER ANNUAL MEETING OF ASME
New Orleans LA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7037, Fax (212) 591-7856, http://www.asme.org

♦ NOVEMBER 24-26, 2002

DIVISION OF FLUID DYNAMICS MEETING OF THE AMERICAN PHYSICAL SOCIETY
Dallas TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 3-7, 2003

MARCH NATIONAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Austin TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 23-27, 2003

225th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
New Orleans LA.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

APRIL 5-8, 2003

APRIL NATIONAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Philadelphia PA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MAY 19-22, 2003

ASME TURBO EXPO
Baltimore MD.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (404) 847-0072, Fax (212) 705-7143, http://www.asme.org

♦ JUNE 8-12, 2003

51st ASMS CONFERENCE ON MASS SPECTROMETRY
Montreal, Canada.

Information: ASMS, 1201 Don Diego Ave., Santa Fe, NM 87505, (505) 989-4517, Fax (505) 989-1073, e-mail: asms@asms.org, http://www.asms.org

♦ JUNE 15-18, 2003

31st NORTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Saratoga Springs NY.

Information: T. Noce, IT Corp., 13 British American Blvd., Latham, NY 12110, (518) 783-6088 ext 283, Fax (518) 783-8397, e-mail: anoce@theitgroup.com

JUNE 22-26, 2003

AIR AND WASTE MANAGEMENT ANNUAL CONFERENCE
San Diego CA.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

♦ SEPTEMBER 7-11, 2003

226th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
New York City NY.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

♦ NOVEMBER 20-22, 2003

55th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Atlanta GA.

Information: H. Hopkins Jr., 5066 Shadow Glen Ct., Atlanta, GA 30338, (770) 396-6265, Fax (404) 636-0453, e-mail: chehph@mindspring.com

CURRENT BIBLIOGRAPHY RELEVANT TO
FUNDAMENTAL COMBUSTION
June 2001

Keith Schofield, ChemData Research, P.O. Box 40481
Santa Barbara, CA 93140, (805) 681-0916, Fax (805) 893-8797
e-mail: combust@mrl.ucsb.edu
http://www.ca.sandia.gov/CRF/Publications/CRB/CRB.html

1. FUELS/SYNFUELS - GENERAL

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Electrospray
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Yields

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Biomass
Heat Content
Analysis

2. LIQUEFACTION/GASIFICATION

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Measurements
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Partial Oxidation

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CH_4/Air
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3. BURNERS

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(88338) Gasification Coals, Chars/CO_2, CO_2/O_2 Mixtures, Measurements, Modeling
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FBC
Ca Sorbents
SO_2 Retention
Mechanism
Issues, Reviews

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Use Potential

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FBC
Low Rank Coals
Ash Agglomeration
Defluidization
Alkali,Sulfur
Roles

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FBC
Coal/Textiles
Co-firing
Economics

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FBC
Coal
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FBC
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Municipal Waste
Co-firing
Cl_2,PCDD/F
Inhibition

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Bubbling FBC
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FBC
Energetic Materials
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CO, CO_2, NO_x Emissions

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FBC
Paper Mill Wastes
Energy Recovery
Demonstrations

4. COAL, PARTICLE COMBUSTION/PYROLYSIS

(See also Section 3 for Coal Burners and Section 21 for Coal Combustion Emissions)

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Coal
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Prospective

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Coal Combustion
Gasification
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Pressure Effects

(88338) Gasification, Circulating Fluidized Bed Measurements, Modeling
Coal/CO_2/O_2
Char/CO_2/O_2

(88337) Gasification, HCl, SO_2 Removal, Efficiencies
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Coal/Biomass
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(88334) Liquefaction, Controlling Factors

Coal/Tire/H_2

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Pulverized Coal/
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Slagging Combustor
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Pulverized Coal/
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Cl_2,HCl
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Gaseous Dominance
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3-Step
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NO Formation

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Activated Carbon
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Combustion
CO_2, $H_2O/O_2/Ar$
Mixtures
Ignition Delays
Burn Times

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Al,Polyethylene
Anthraquinone Dusts

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Combustion
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Flow
Modeling

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α-HMX
Unimolecular
Dissociation
Channels
Rate Constants
Calculations

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HMX

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Explosive Materials

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Soot
Modeling

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Thin Cellulose

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Natural Gas
Combustion
High Pressure
Turbine Conditions
NO_x Formation

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Catalytic
CH_3OH/O_2

(88342) Partial Oxidation to HCHO, Yields, Model, Optimal Control

Catalytic
CH_3OH/O_2

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Dynamics
Measurements

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Oxidation
$CO/O_2/RuO_2$
Reactivity

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Efficiencies

8. MHD

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Rotational
N_2,Air Plasmas

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Temperatures

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Rapid Compression Cylinder
$(t\text{-}C_4H_9)_2O_2$

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High Pressures
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Rotational
T,N_2,O_2
Single Shot Measurements
300-773 K
1-50 bar

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Temperatures
CARS

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Modeling

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2-D Raman
CH_4 Density
Measurements

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Lengths
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CO,NO Emissions

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Strain Rate
Disturbances
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Measurements
Model Deficiencies

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Modeling

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(88817)	Turbulent Flows, Kinetic Modeling, Pressure Effects	C_3H_8/O_2
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CH_4, C_3H_8/Air
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Measurements

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In-situ Formation

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Air
2-D Modeling
New Hybrid Scheme

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Supersonic Flows
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Flame/Stretch
Interactions
Measurements
H,OH Role

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15. IONIZATION

(See also Section 26 for Ion Spectroscopy, Section 27 for Ion Lifetimes and Penning Ionization, Section 40 for Dynamics of Ion-Molecule Reactions, Section 42 for REMPI, Section 43 for P.E. Surfaces and Energy Levels, Section 44 for Ionic Structures and Section 46 for Thermochemical Values)

(88788)	Double Focusing Instruments, Review	ICP/Mass Analysis
(88787)	CH_3OOH, H_2O_2 , Atmospheric Mass Analysis Method	Chemical Ionization Monitor
88458.	MacTaylor, R.S., and A.W. Castleman, Jr., "Cluster Ion Reactions: Insights into Processes of Atmospheric Significance," *J. Atm. Chem.* 36, 23-63 (2000).	Ion Cluster Reactions Atmospheric Species HCl,HNO_3,N_2O_5,$ClONO_2$ O^-,HO_2^-,OH^- Water Clusters Rate Constants
88459.	Datz, S., "Dynamics of Dissociative Recombination of Molecular Ions: Three-Body Breakup of Triatomic Dihydrides," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 2369-2373 (2001).	$MH_2^+ + e^-$ 3-Product Fragmentation Dynamics Calculations
88460.	Groenewold, G.S., B.D.M. Hodges, J.R. Scott, A.K. Gianotto, A.D. Appelhans, G.F. Kessinger and J.B. Wright, "Oxygen-for-Sulfur Exchange in the Gas Phase: Reactions of Al and Si Oxyanions with H_2S," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 4059-4064 (2001).	$AlO_2^- + H_2S$ $SiO_2^- + H_2S$ $SiO_3^- + H_2S$ Channels
(88644)	Clusters, Photoelectron Spectra, Transition State Behavior	$BrHI^-$.Ar IHI^-.Ar
(89101)	Vibrational Relaxation, Radiative Lifetimes, Measurements/Theory, Discrepancies	$DCO^+(1,2\nu_{CD})$ $DCO^+(\nu_{CO})$

88461.	Dose, V., P. Pecher and R. Preuss, "Formulas for Cross Sections and Rate Coefficients for Partial Electron Impact Ionization of CH_4 and H_2," *J. Phys. Chem. Ref. Data* 29, 1157-1164 (2000).	$CH_4, H_2 + e^-$ Ionization Cross Sections Rate Constants
88462.	Cacace, F., G. de Petris, M. Rosi and A. Troiani, "Ionization of Atmospheric Gases Containing Ozone and Carbonyl Sulfide: Formation and Reactivity of SO^+ Ions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1144-1149 (2001).	OCS/O_3 Ionization SO^+ Product Ions
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(88645)	Clusters, Photoionization Induced CH_4 Formation, Measurements	$(C_2H_4)_m(NO)_n$
88466.	Chen, Y.-J., P.T. Fenn and C.Y. Ng, "Direct Identification of Product CH_2SH^+/CH_3S^+ Structures in the Dissociation of $CH_3CH_2SH^+$ and $CH_3SCH_3^+$ via Collisional Activation," *Chem. Phys. Lett.* 336, 105-108 (2001).	$C_2H_5SH^+ + Ar$ $(CH_3)_2S^+ + Ar$ Dissociation CH_3S^+, CH_2SH^+ Product Ions
88467.	Fairley, D.A., D.B. Milligan, L.M. Wheadon, C.G. Freeman, R.G.A.R. Maclagan and M.J. McEwan, "Flow Tube and Theoretical Study of Proton Transfer Reactions of $C_3H_5^+$ Ions," *Int. J. Mass Spectrom. Ion Process.* 185/186/187, 253-261 (1999).	$CH_2CHCH_2^+ + M$ $CH_3CCH_2^+ + M$ Rate Constants Isomeric Ion Monitoring Method Isomerization Energy
88468.	Fialkov, A.B., J. Dennebaum and K.-H. Homann, "Large Molecules, Ions, Radicals and Small Soot Particles in Fuel-Rich Hydrocarbon Flames. V. Positive Ions of Polycyclic Aromatic Hydrocarbons in Low Pressure Premixed Flames of Benzene and Oxygen," *Combust. Flame* 125, 763-777 (2001).	PAH Cations Low Pressure C_6H_6/O_2 Mass Analysis Profiles
(88801)	LIF/Probe Measurements, Cl_2 Discharges	Cl^+, Cl_2^+
(88964)	Reaction Dynamics, Cluster Effects	$Cl^-(H_2O) + CH_3Br$

		$Cl^-(H_2O)_2+CH_3Br$
88469.	Amelynck, C., C. Stepien, N. Schoon, V. Catoire, D. Labonnette, E. Arijs and G. Poulet, "Gas Phase Reactions of Negative Ions with $ClONO_2$," *Int. J. Mass Spectrom. Ion Process.* 207, 205-215 (2001).	$ClONO_2+B^-$ Rate Constants B=F,Cl,Br,I, NO_2,NO_3,SF_6, CO_3,CO_4 Measurements
(89004)	Discharge, Ions/Neutrals, Product Modeling	Cl_2/O_2
(88802)	LIF, ICP, Plasma Measurements	Cl_2^+
88470.	Deutsch, H., K. Becker and T.D. Mark, "Application of the Deutsch/Mark Formalism to the Calculation of Electron-Impact Ionization Cross Sections of Alkali Atoms," *Int. J. Mass Spectrom. Ion Process.* 185/186/187, 319-326 (1999).	e^-+Alkali Atoms Ionization Cross Sections Formalism
88471.	Deutsch, H., K. Becker, S. Matt and T.D. Mark, "Theoretical Determination of Absolute Electron-Impact Ionization Cross Sections of Molecules," *Int. J. Mass Spectrom. Ion Process.* 197, 37-69 (2000).	e^-+Molecule Ionization Cross Sections 31 Cases Theoretical Method
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88473.	Stebbings, R.F., and B.G. Lindsay, "Comment on the Accuracy of Absolute Electron-Impact Ionization Cross Sections for Molecules," *J. Chem. Phys.* 114, 4741-4743 (2001).	e^- Impact Cross Sections H_2,CO,CH_4,N_2 CO_2,SF_6,O_2,NO Experimental Comparisons
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(88965)	Reaction Dynamics, Collision Energy Dependence, Cluster Effects, Channels, Branching Ratios	$F^-(H_2O)+CH_3Cl$

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$HOCO^+$
Isomerization
Dissociation
Dynamics
HCO^+ Product Channel

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$H_2(v)+e^-$
Dissociative Attachment
v,J Effects

88477. Rosen, S., A. Derkatch, J. Semaniak, A. Neau, A. Al-Khalili, A. Le Padellec, L. Vikor, R. Thomas, H. Danared, M. af Ugglas and M. Larsson, "Recombination of Simple Molecular Ions Studied in Storage Ring: Dissociative Recombination of H_2O^+," *Faraday Discuss. Chem. Soc.* 115, 295-302 (2000).

$H_2O^+ + e^-$
Dissociative Recombination
Cross Sections
Branching Ratios

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$H_3O^+ + e^-$
$H_3O^+ + Cl^-, Br^-, I^-$
Dissociative Recombination
Rate Constants
Flame Measurements

88479. Spanel, P., and D. Smith, "Selected Ion Flow Tube Studies of the Reactions of H_3O^+, NO^+ and O_2^+ with Some Chloroalkanes and Chloroalkenes," *Int. J. Mass Spectrom. Ion Process.* 184, 175-181 (1999).

$H_3O^+ + RCl$
$NO^+, O_2^+ + RCl$
8 Chloroalkanes
2 Chloroethylenes
Rate Constants
Product Ions

88480. Spanel, P., and D. Smith, "Selected Ion Flow Tube Studies of the Reactions of H_3O^+, NO^+ and O_2^+ with Several Aromatic and Aliphatic Monosubstituted Halocarbons," *Int. J. Mass Spectrom. Ion Process.* 189, 213-223 (1999).

$H_3O^+ + RX$
$NO^+, O_2^+ + RX$
Rate Constants
Ion Products

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$He_2^+(v,J) + e^-$
Rate Constants
Isotopes
P.E. Curves
Mechanism
Calculations

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$Kr^+(^2P_{1/2,3/2})$
$Xe^+(^2P_{1/2,3/2})$
Spin-Orbit State Monitoring
Ion Mobility
Mass Analysis Method

88483.	Chen, Q.-F., and J.M. Goodings, "Chemical Kinetics of Lanthanum Ionization in $H_2/O_2/N_2$ Flames," *Int. J. Mass Spectrom. Ion Process.* 188, 213-224 (1999).	La Flame Ionization Chemistry LaO^+,$LaO^+(H_2O)$ Mass Analysis
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(88768)	108 Transition Probabilities, Visible Spectral Region	N^+
88485.	Ijjaali, F., M. El-Mouhtadi, M. Esseffar, M. Alcami, O. Mo and M. Yanez, "The Role of Spin-Forbidden Processes in $N^+(^3P)+NH_3$ Reactions in the Gas Phase," *Phys. Chem. Chem. Phys.* 3, 179-183 (2001).	N^++NH_3 ^{1,3}P.E. Surfaces Nonadiabatic Crossing Mechanism Role
(89111)	Vibrational Relaxation, Rate Constants, Measurements	$NO^+(v=1,4)+CH_4$
88486.	Midey, A.J., S. Williams and A.A. Viggiano, "Reactions of NO^+ with Isomeric Butenes from 225 to 500 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1574-1578 (2001).	$NO^++C_4H_8$ 4 Butene Isomers Rate Constants Branching Ratios
88487.	Tosi, P., W. Lu, D. Bassi and R. Tarroni, "The Reaction $N_2^++N_2 \rightarrow N_3^++N$ from Thermal to 25 eV," *J. Chem. Phys.* 114, 2149-2153 (2001).	$N_2^++N_2$ Reactive Cross Sections Energy Dependence
88488.	Fishman, V.N., S.T. Graul and J.J. Grabowski, "Selected Ion Flow Tube Studies of the Atomic Oxygen Radical Cation Reactions with Ethylene and Other Alkenes," *Int. J. Mass Spectrom. Ion Process.* 185/186/187, 477-496 (1999).	$O^++C_2H_4$ O^++Alkenes Channels Branching Ratios Product Ions
88489.	Stancil, P.C., K. Kirby, J.-P. Gu, G. Hirsch, R.J. Buenker and A.B. Sannigrahi, "The Formation of SiH^+, PH^+ and SH^+ by Radiative Association," *Astron. Astrophys., Suppl. Ser.* 142, 107-112 (2000).	P^++H S^+,Si^++H Radiative Association Cross Sections Calculations
88490.	Tachikawa, H., and T. Yamano, "A Full Dimensional Direct ab Initio Dynamics Study of the Electron Capture by SF_6," *Chem. Phys.* 264, 81-89 (2001).	SF_6+e^- Dissociative Attachment Dynamics Theory

88491. Catoire, V., C. Stepien, D. Labonnette, J.-C. Rayez, M.-T. Rayez and G. Poulet, "Kinetics of the Reaction of SF_6^- with O_3," *Phys. Chem. Chem. Phys.* 3, 193-197 (2001).

$SF_6^- + NO_2, O_3, Cl_2$
$O_2^- + O_3$
$CO_4^- + O_3$
Rate Constants

88492. Arnold, S.T., and A.A. Viggiano, "Turbulent Ion Flow Tube Study of the Cluster-Mediated Reactions of SF_6^- with H_2O, CH_3OH and C_2H_5OH from 50 to 500 torr," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3527-3531 (2001).

$SF_6^-.ROH + ROH$
Rate Constants
$R = CH_3, C_2H_5, H$
Product Ions

(89012) Optical Frequency Standards, Magnetic Field Independence

$Sr^+(^2D_{5/2}-^2S_{1/2})$

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$V^+, VO^+ + O_2$
$V^+, VO^+ + H_2O$
Rate Constants
Measurements
Mechanisms

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$Zr^+, ZrO^+ + CO_2$
$ZrO^+, ZrO_2^+ + CO$
Ion Beam
Measurements
$D_0(ZrO_2^+)$
$D_0(Zr^+CO_n), n = 1\text{-}3$

16. INHIBITION/ADDITIVES

(See also Section 21 for Combustion Emission Control Additives)

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CO_2 Additive
C_2H_4 Diffusion
Counterflow
Flame
Soot,NO
Effects

(88352) SO_2 Retention, FBC, Mechanism, Issues, Review

Ca Sorbents

88496. Oxley, J.C., J.L. Smith, E. Rogers, W. Ye, A.A. Aradi and T.J. Henly, "Fuel Combustion Additives: A Study of Their Thermal Stabilities and Decomposition Pathways," *Energy Fuels* 14, 1252-1264 (2000).

Fuel Additives
Cetane Improvers
Nitrates,Peroxides
$Mn(CO)_3$
Major Dissociation
Roles

(88447) Inerting Additives, Al(s), Polyethylene, Anthraquinone Dusts, Explosion Suppression

$(NH_4)H_2PO_4, NaHCO_3$

88497. MacDonald, M.A., F.C. Gouldin and E.M. Fisher, "Temperature Dependence of Phosphorus Based Flame Inhibition," *Combust. Flame* 124, 668-683 (2001).

Inhibition
Organophosphates
$CH_4/O_2/N_2, Ar$

DMMP
Mechanism

88498. Korobeinichev, O.P., T.A. Bolshova, V.M. Shvartsberg and A.A. Chernov, "Inhibition and Promotion of Combustion by Organophosphorus Compounds Added to Flames of CH_4 or H_2 in O_2 and Ar," *Combust. Flame* 125, 744-751 (2001).

Inhibition
Organophosphates
$CH_4/O_2/Ar$
$H_2/O_2/Ar$
Species Profiles
Kinetic Modeling

(88357) PCDD/F, Cl_2 Inhibition, FBC, High S/Cl Coal/Municipal Waste Cofiring — SO_2 Effects

(88638) H_2/O_2 Flame Additive, SiO Formation/Decay, LIF Measurements — $(Si(CH_3)_3)_2NH$

(88639) CH_4/O_2 Flame Additive, TiO_2 Particle Formation, Growth, Coagulation — $Ti(C_3H_7O)_4$

17. CORROSION/EROSION/DEPOSITION

(See also Section 22 for Diamond Formation Deposition)

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Deposition
Hot Flue Gases
Cleanup
Particulates
Formation
Composition

88500. Andersen, K.H., F.J. Frandsen, P.F.B. Hansen, K. Wieck-Hansen, I. Rasmussen, P. Overgaard and K. Dam-Johansen, "Deposit Formation in a 150 MW_e Utility Pulverized Fuel Boiler During Co-combustion of Coal and Straw," *Energy Fuels* 14, 765-780 (2000).

Deposition
K_2SO_4
KAl Silicate
Coal/Straw
Cofired Boiler
Testing

18. GAS/SURFACE INTERACTIONS/BOUNDARY LAYER COMBUSTION

(See also Section 7 for Catalytic Combustion, Section 17 for Deposition Processes, Section 21 for Emission Control Sorbents and Section 22 for Particle Formation and Deposition)

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Fire Dynamics
Flammability
Spread, Ignition
Smoldering
Handbook

88502. Evans, D.D., G.W. Mulholland, H.R. Baum, W.D. Walton and K.B. McGrattan, "In-Situ Burning of Oil Spills," *J. Res. Natl. Inst. Stand. Technol.* 106, 231-278 (2001).

Oil Spill
Burning
In-Situ
Response Method

88503. Walavalkar, A.Y., and A.K. Kulkarni, "Combustion of Water-in-Oil Emulsion Layers Supported on Water," *Combust. Flame* 125, 1001-1011 (2001).

Oil/Water
Emulsion
Floating on Water
Combustion
Measurements
Modeling

88504. Olson, S.L., T. Kashiwagi, O. Fujita, M. Kikuchi and K. Ito, "Experimental Observations of Spot Radiative Ignition and Subsequent Three-Dimensional Flame Spread over Thin Cellulose Fuels," *Combust. Flame* 125, 852-864 (2001).

Flame Spread
Thin Cellulose
Radiative Ignition
Microgravity
Measurements

88505. Wu, J., J. Seyed-Yagoobi and R.H. Page, "Heat Transfer and Combustion Characteristics of an Array of Radial Jet Reattachment Flames," *Combust. Flame* 125, 955-964 (2001).

Radial Jet
Impingement
Flame Heating
Nozzle Array
Heat Transfer

88506. Poschl, U., T. Letzel, C. Schauer and R. Niessner, "Interaction of Ozone and Water Vapor with Spark Discharge Soot Aerosol Particles Coated with Benzo[*a*]pyrene: O_3 and H_2O Adsorption, Benzo[*a*]pyrene Degradation and Atmospheric Implications," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 4029-4041 (2001).

Heterogeneous
Interactions
Soot/PAH Coated
H_2O,O_3
Mechanisms

88507. Turner, C.H., J.K. Johnson and K.E. Gubbins, "Effect of Confinement on Chemical Reaction Equilibria: The Reactions $2NO \leftrightarrow (NO)_2$ and $N_2+3H_2 \leftrightarrow 2NH_3$ in Carbon Micropores," *J. Chem. Phys.* 114, 1851-1859 (2001).

Heterogeneous
Carbon Micropores
$2NO/(NO)_2$
$N_2+3H_2/2NH_3$
Equilibrations
Simulations

88508. Zangmeister, C.D., and J.E. Pemberton, "Raman Spectroscopy of the Reaction of Sodium Chloride with Nitric Acid: Sodium Nitrate Growth and Effect of Water Exposure," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3788-3795 (2001).

Heterogeneous
HNO_3/NaCl(s)
$NaNO_3$ Growth
Monitoring
H_2O Effects

88509. Lefevre, L., T. Belmonte and H. Michel, "Modeling of Nitrogen Atom Recombination on Pyrex: Influence of the Vibrationally Excited N_2 Molecules on the Loss Probability of N," *J. Appl. Phys.* 87, 7497-7507 (2000).

Heterogeneous
Recombination
N/Pyrex
Rate Constants
Measurements
Mechanism

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Heterogeneous
Recombination

N,O Atoms
Stainless Steel
Coefficients

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Heterogeneous
NO/Rh(s)
Reduction
N_2 Product
N_2O Intermediate
Role

88512. Gordiets, B., C.M. Ferreira, M.J. Pinheiro and A. Ricard, "Self-Consistent Kinetic Model of Low Pressure N_2-H_2 Flowing Discharges. II. Surface Processes and Densities of N, H, NH_3 Species," *Plasma Sources Sci. Technol.* 7, 379-388 (1998).

Surface Processes
N_2/H_2 Discharges
N,H Formation
Radical Wall Loss
Probabilities
Model

88513. Guo, X.-Y., and F.J. Keil, "Kinetics of N_2O Catalytic Decomposition over Three-Dimensional Fractals," *Chem. Phys. Lett.* 330, 410-416 (2000).

Catalytic
Decomposition
N_2O
Fractal Surface
Effects
Modeling

19. ENGINES/EMISSIONS

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I.C. Engine
Pent-roof Cylinder
CFD Modeling
Flowfield

88515. Kim, W.T., K.Y. Huh, J.W. Lee and K.Y. Kang, "Numerical Simulation of Intake and Compression Flow in a Four Valve Pent-roof Spark Ignition Engine and Validation with LDV Data," *Proc. Inst. Mech. Eng. D. J. Auto Eng.* 214, 361-372 (2000).

I.C. Engine
Pent-roof Cylinder
LDV Flowfield

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Gas Turbines
Nonperfect Gas
Effects
Modeling
Optimization

88517. Mansouri, S.H, and Y. Bakhshan, "The k-ε Turbulence Modeling of Heat Transfer and Combustion Processes in a Texaco Controlled Combustion Stratified Charge Engine," *Proc. Inst. Mech. Eng. D. J. Auto Eng.* 214, 149-158 (2000).

Stratified
Charge Engine
Turbulence
Model
Data Comparisons

88518. Lee, Y., S. Pae, K. Min and E.S. Kim, "Prediction of Knock Onset and the Auto-ignition Site in Spark Ignition Engines," *Proc. Inst. Mech. Eng. D. J. Auto Eng.* 214, 751-763 (2000).

I.C. Engines
Auto-ignition
Turbulent/

Chemical Kinetic Model

88519. Yossefi, D., S.J. Maskell, S.J. Ashcroft and M.R. Belmont, "Ignition Source Characteristics for Natural Gas Burning Vehicle Engines," *Proc. Inst. Mech. Eng. D. J. Auto Eng.* 214, 171-180 (2000).
I.C. Engines
Natural Gas
Ignition Source
Assessments
Modeling

88520. Wang, W., E.C. Chirwa, E. Zhou, K. Holmes and C. Nwagboso, "Fuzzy Ignition Timing Control for a Spark Ignition Engine," *Proc. Inst. Mech. Eng. D. J. Auto Eng.* 214, 297-306 (2000).
I.C. Engine
Ignition Timing
Fuzzy Logic
Theory
Control Method

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Soot,NO_x
Emissions

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Measurements

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Equilibrium
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Modeling

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(88373)	Coal Char Combustion, HNCO Detection, 600 °C Measurements	NO Formation
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(88427)	Turbulent Combustion Modeling, Natural Gas Furnace	NO Formation
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(88383)	Heavy Oil Combustion, H_2O Emulsions, Spray Dependence	NO_x, Soot Emissions
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NO,N_2O
Formation,Control
Mechanisms
Staged Combustion
Dependences

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N_2O
Formation/
Destruction
Coal Combustion
Preheating,Staging
Reburn Effects

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N_2O Formation
Destruction
Coal Combustion
Kinetic Modeling
Dependences

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NO_x Control
Impinging Jet
Flame
Chamber Geometry
Effects

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NO Control
Wood Combustion
Staging,FGR
Methods

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O_2 Enriched Air
Combustion
Staging Controls

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NO Control
Gas Turbines
Staging
Biomass Syngas
Kinetic Modeling

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NO_x,N_2O Control
Circulating FBC
T,Air Staging Effects

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2-Stage FBC
Limestone Feed Effects

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NO_x Control
Low O_2 Combustion Approach

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Pulsed Flow
Acoustic Methods

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UV,Pulsed Discharge Method

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CO/O_2/Catalyst Method
C_3H_6,C_3H_8 Effects

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Hydrocarbon/ Catalyst Method
RH Structure Effects
Efficiencies

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Na,K,Ca,Fly Ash
Additive Effects
SO_2 Reductions

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N_2O Control
C_3H_6/O_2/Catalyst Method
Induction Period
Mechanism

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N_2O Control
Microwave Discharge
Efficiencies
N_2O/He,Ar

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SO_2 Emission

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NO,SO_2 Control
Flue Gases
e^--Beam Method
Oxidation
Kinetic Model
H_2O,H_2SO_4
Condensation

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SO_2 Control
e^--Beam Method
Flue Gases
H_2O,H_2SO_4
Condensation
Modeling

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SO_2 Control
Flue Gas
Cleanup Methods

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SO_2 Control
High Current
Photodischarge
Method
Efficiencies

22. SOOT, DIAMOND, PARTICLE FORMATION/CONTROL

(See also Section 19 for Engine Soot Formation)

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(88495)	C_2H_4 Diffusion Counterflow Flame, CO_2 Additive Effects on Soot, NO Formation	Soot Formation
88631.	Hwang, J.Y., and S.H. Chung, "Growth of Soot Particles in Counterflow Diffusion Flames of Ethylene," *Combust. Flame* 125, 752-762 (2001).	Soot Growth PAH Coagulation Counterflow C_2H_4 Diffusion Measurements Modeling
(88392)	Polymer Combustion, Emissivity, Modeling	Soot Formation

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Soot Yields
Growth
Plug Flow Reactor
Turbulent
Jet Diffusion
Flame

(88789) $CH_4/H_2/Ar$, C_2(d-a) Emission/Absorption Comparison Measurements

Diamond Formation

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Diamond Formation
C_2H_2/O_2 Flame
CN Role
LIF Measurements
N_2 Addition
Effects

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Diamond Formation
$CH_4/H_2/CO$
$CH_4/H_2/O_2$
Discharges
C,O,OH Roles
Mechanisms

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Diamond Formation
Raman Spectra
244,325,514 nm
Excitation
Comparisons
Peak Intensities

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Al_2O_3,ZrO_2
Nanoparticle
Formation Method
Aerosol/Flame
Sizes

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Fe_2O_3
Nanoparticles
$H_2/O_2/Ar$
Flame Formation
Sizes

(88367) Conversion Rates, Particulate Sizes, Coal Fired Power Plant Plume Emissions, FGD Controls

SO_2/SO_4^{2-}

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SiO
Formation/
Decay
LIF
H_2/O_2 Flames

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23. PARTICLE CHARACTERIZATION

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(88382)	Fine Emission Particles, Sizes, Fuel Oil Combustion	Trace Element Content
88641.	Liu, K., W. Xie, D. Li, W.-P. Pan, J.T. Riley and Al Riga, "The Effect of Chlorine and Sulfur on the Composition of Ash Deposits in a Fluidized Bed Combustion System," *Energy Fuels* 14, 963-972 (2000).	Ash FBC Cl,S Retention Analysis
(88354)	FBC, Low Rank Coals, Defluidization, Alkali, Sulfur Roles	Ash Agglomeration
(88369)	Coal Combustion, Trace Minerals, Volatiles, Measurements	Ash Analysis
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(88368)	Sizes, Trace Elements, Pulverized Coal, Fuel Oil Combustion, Measurements	Particle Emissions
(88575)	Biomass Combustion, Composition Types	Particle Emissions
(88786)	Laser Method	Small Particle Monitoring

24. NUCLEATION/COAGULATION/CLUSTERS

(See also Section 22 for Particle Formation and Section 44 for Cluster Structural Calculations)

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(88458)	O^-, HO_2^-, OH^- Water Clusters, Reactions with HCl, HNO_3, N_2O_5, $ClONO_2$, Rate Constants	Atmospheric Ion Clusters
(89120)	Photodissociation Spectrum, D_0, Measurements	Al_3, V_3^+
88644.	Liu, Z., H. Gomez and D.M. Neumark, "Photoelectron Spectroscopy of Clustered Transition State Precursors $IHI^-.Ar$ and $BrHI^-.Ar$," *Chem. Phys. Lett.* 332, 65-72 (2000).	$BrHI^-.Ar$ $IHI^-.Ar$ Clusters Photoelectron Spectra Transition State Behavior
(88737)	Predissociation Lifetimes, Product Rotational Distributions, Modeling	$Br_2(B).He$
88645.	DeLeon, R.L., E.F. Rexer and J.F. Garvey, "Photochemical Generation of Methane within NO-Ethene Heteroclusters," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 2266-2269 (2001).	Clusters $(C_2H_4)_m(NO)_n$ Photoionization Induced CH_4 Formation
(89043) (89044)	Comment and Reply on the Interaction Potential, Theoretical Description	$(CO)_2$
(89015)	Product Ions, Graphite Laser Ablation, TOF Mass Analysis, Two Component Plume	C_n^+
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(89139)	Review of Experimental and Theoretical Data	$D(C_{58}-C_2)$
(89028)	MPI, fs Pulsed Laser, Sequential Ionization	C_{60}
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(88919) Unimolecular Decay, P.E. Surface, Symmetry Specific Effects, Calculations — $Cl^-.CH_3Cl$

(88964) Reaction Dynamics, Cluster Effects — $Cl^-(H_2O)+CH_3Br$; $Cl^-(H_2O)_2+CH_3Br$

(88965) Reaction Dynamics, Collision Energy Dependence, Cluster Effects, Channels, Branching Ratios — $F^-(H_2O)+CH_3Cl$

(89110) Predissociation, Vibrational Relaxation, fs Pump/Probe Monitoring, B/a State Coupling — $I_2(B).Rg_n$

(89061) P.E. Surfaces, Vibrational Levels, Infrared Spectral Predictions — NO.Ne

(88882) Photodetachment, Hydration Energies, Mechanisms — $O_2^-(H_2O)_{1\text{-}6}+h\nu$

25. FLAME/CHEMILUMINESCENT SPECTROSCOPY

26. SPECTRAL CHARACTERIZATIONS/ANALYSES

(See also Section 43 for Energy Levels and Theoretically Calculated Spectral Constants, and Section 44 for Vibrational Frequencies and Constants)

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FTIR Spectra
Assignments
Matrix Study

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AuCl,AuBr
Rotational
Spectra
Constants
Ionic Degree

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Emission Spectrum
Assignments

(88644) Cluster Photoelectron Spectra, Transition State Behavior
$BrHI^-$.Ar
IHI^-.Ar

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BrO_2

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(88850)	Ultraviolet Spectrum, Measurements	$CH_3CH(OH)O_2$
(89132)	Photoionization Efficiency Spectrum, IP(CH_3SCH_2 ,CH_3SCH_2Cl), Measurements	CH_3SCH_2Cl
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Lifetimes
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Constants
Energies

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Spectral Constants

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Rotational
Spectra
Constants
Geometries

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(89017)	Product FTIR Spectrum, Laser Ablation, U(s)/N_2, Matrix Study	UN
88729.	Ram, R.S., P.F. Bernath and S.P. Davis, "Fourier Transform Infrared Emission Spectroscopy of VCl," *J. Chem. Phys.* 114, 4457-4460 (2001).	VCl($^5\Delta$-$X^5\Delta$) FTIR Spectra Constants
88730.	Gullberg, D., and U. Litzen, "Accurately Measured Wavelengths of Zn and Zn^+ Lines of Astrophysical Interest," *Phys. Scr.* 61, 652-656 (2000).	Zn,Zn^+ Energy Level Refinements FT Spectra
88731.	Ram, R.S., A.G. Adam, W. Sha, A. Tsouli, J. Lievin and P.F. Bernath, "The Electronic Structure of ZrCl," *J. Chem. Phys.* 114, 3977-3987 (2001).	ZrCl(E,C-X) ZrCl(d-a) Electronic Spectral Reassignments

27. EXCITED STATE LIFETIMES/QUENCHING

(See also Section 45 for Vibrational and Rotational Relaxation Processes)

88732.	Trabert, E., "Atomic Lifetime Measurements with Ion Traps of Many Sizes," *Phys. Scr.* 61, 257-286 (2000).	Atomic Ions Lifetimes Ion Trap Capabilities
88733.	Molisch, A.F., B.P. Oehry and G. Magerl, "The Influence of Radiation Trapping on the Measurements of Cross Sections for Excited Atom/Excited Atom Collisions," *Phys. Scr. Colloq.* T86, 55-61 (2000).	A*+A* Cross Sections Radiation Trapping Effects Model
88734.	Brunetti, B.G., P. Candori, S. Falcinelli, T. Kasai, H. Ohoyama and F. Vecchiocattivi, "Velocity Dependence of the Ionization Cross Section of Methyl Chloride Molecules Ionized by Metastable Argon Atoms," *Phys. Chem. Chem. Phys.* 3, 807-810 (2001).	Ar*+CH_3Cl Penning Ionization Cross Sections Energy Dependence Crossed Beams

88735. Matsuo, Y., T. Nakajima, T. Kobayashi and M. Takami, "Radiative Lifetimes and Collisional Deactivation Cross Sections of the 5d6p States of Laser Ablated Ba in He Gas," *Phys. Rev. A: At. Mol. Opt. Phys.* 59, 2071-2077 (1999).

$Ba(5d6p\ ^3P)$
$Ba(5d6p\ ^3D,^3F)$
$Ba(5d^2\ ^3P_2)$
Radiative Lifetimes
He Quenching Cross Sections
Measurements

88736. Derkatch, A., C. Lundevall, L.-E. Berg and P. Royen, "Lifetime Measurements of the $A^2\Pi$ State of BaCl Using Laser Spectroscopy," *Chem. Phys. Lett.* 332, 278-282 (2000).

$BaCl(A^2\Pi_{1/2,3/2})$
Radiative Lifetimes
Measurements

88737. Jung, J., and H. Sun, "The Vibrational Structure and Predissociation of the B-State of $HeBr_2$ Using a Simple Theoretical Method," *Chem. Phys. Lett.* 336, 311-320 (2001).

$Br_2(B).He$
Predissociation
Lifetimes
Product J Distributions
Modeling

88738. Metropoulos, A., and A. Mavridis, "Predissociation Lifetimes of the $E^2\Pi$ and $F^2\Pi$ States of CH," *Chem. Phys. Lett.* 331, 89-94 (2000).

CH(F,E)
Predissociation
Lifetimes
Calculations

(89113) Rotational Energy Transfer, State-to-State Cross Sections, Measurements, Calculations

CH(A,v=0,J)+Ar

88739. Wysong, I.J., "Measurement of Quenching Rates of $CO(a^3\Pi,v=0)$ Using Laser Pump-and-Probe Technique," *Chem. Phys. Lett.* 329, 42-46 (2000).

CO(a,v=0)+M
Quenching
Rate Constants
M=6 Gases

88740. Karlsson, H.O., "Predissociation Resonances in CO and IBr: Smooth Exterior Scaling Combined with the Discrete Variable Representation," *Eur. Phys. J. D* 11, 207-212 (2000).

CO(B/D′)
IBr(B/Y)
Interactions
Predissociation Resonances
Calculations

88741. Di Teodoro, F., and R.L. Farrow, "$CO^+(B^2\Sigma^+,v=0)$ Emission Induced by Laser Excitation of Neutral CO at 230 nm," *J. Chem. Phys.* 114, 3421-3428 (2001).

$CO^+(B)+M$
Quenching
Rate Constants
9 Collider Species
(2+1) REMPI
CO Pumping

(88945) Reaction Dynamics, Rate Constants, Barrier Height, Calculations, Data Comparisons

$C_2(a)+H_2$

88742. Makarov, V.I., A.R. Cruz and E. Quinones, "Collisional Nature of the Magnetic Field Quenching of the Acetylene A^1A_u State," *Chem. Phys.* 264, 101-110 (2001).

$C_2H_2(A^1A_u)$
LIF
Magnetic Quenching
^{1,3}Intersystem
Crossing Effects

88743. Nagai, H., R.T. Carter and J.R. Huber, "Spectroscopy and Dynamics of Selected Rotational Levels in the B^2A'' State of the Vinoxy Radical," *Chem. Phys. Lett.* 331, 425-432 (2000).

$CH_2CHO(B,v,J)$
Single Rotational
Level
Lifetimes
Measurements

(88956) Reaction Dynamics, Pathways, Energetics, Calculations

$Cd(^1P,^3P,^1S)+GeH_4$
$Hg(^1P,^3P,^1S)+GeH_4$

88744. Nakao, Y., K. Hirao and T. Taketsugu, "Theoretical Study of the Water Activation by a Cobalt Cation: Ab Initio Multireference Theory Versus Density Functional Theory," *J. Chem. Phys.* 114, 5216-5223 (2001).

$Co^+(^5F)+H_2O$
$Co^+(^3F)+H_2O$
Channels
CoH^+,CoO^+ States
D_0 ,r_e
Energies

(88897) Spin-Orbit Splitting Role, $F+n$-H_2 Cross Sections, Crossed Beam Measurements, HF(v=3,J) Product

$F(^2P_{1/2})+n$-H_2

88745. Korolkov, M.V., and K.-M. Weitzel, "The Spin-Orbit Induced Predissociation Dynamics of HCl^+ Ions: Rotational Islands of Stability," *Chem. Phys. Lett.* 336, 303-310 (2001).

$HCl^+(A,v,N)$
Predissociation
Lifetimes
Rotationally
Stable Regions
Calculations

88746. Imura, K., N. Kishimoto and K. Ohno, "Two-Dimensional Penning Ionization Electron Spectroscopy of Monohalogenobenzenes by $He(2^3S)$: C_6H_5X(X=F, Cl, Br, I)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 4189-4199 (2001).

$He(2^3S)+C_6H_5X$
X=F,Cl,Br,I
Penning Ionization
Cross Sections
Mechanism

88747. Ohno, K., M. Yamazaki, N. Kishimoto, T. Ogawa and K. Takeshita, "Trajectory Calculations of Two-Dimensional Penning Ionization Electron Spectra of N_2 in Collision with Metastable $He(2^3S)$ Atoms," *Chem. Phys. Lett.* 332, 167-174 (2000).

$He(2^3S)+N_2$
Penning Ionization
Cross Sections
N_2(B,A,X) Channels
Calculations

88748. Blagoev, K., R. Roussev, A. Morozov, K. Iskra and L. Windholz, "Radiative Lifetimes of (7d,8d $^1D_2$) Excited States of Hg," *Eur. Phys. J. D* 13, 159-163 (2001).

Hg(7,8d $^1D_2$)
Radiative
Lifetimes

88749. Akopyan, M.E., N.K. Bibinov, D.B. Kokh, A.M. Pravilov, O.L. Sharova and M.B. Stepanov, "The Approach-Induced $I_2(E0_g^+ \rightarrow D0_u^+)$ Transitions, M=He, Ar, I_2, N_2, CF_4," *Chem. Phys.* 263, 459-470 (2001).

I_2(E/D)
Collision Induced
Transition
5 Collision Partners

		Cross Sections Propensity Rules
(89110)	Predissociation, B/a State Coupling, Vibrational Relaxation, fs Pump/Probe	$I_2(B).Rg_n$
88750.	Schoon, N., and E. Desoppere, "Experimental and Theoretical Study of the Imprisonment of the $Kr(^3P_1$-$^1S_0)$, 123.58 nm Resonance Radiation," *J. Quant. Spectrosc. Radiat. Transfer* 67, 199-216 (2000).	$Kr(^3P_1)$ Lifetime Lineshapes Imprisonment Cell
(88982)	Reaction Dynamics, Transition State, P.E. Surfaces, Decay Channels, Calculations	$Li(^2P).HF$
(89099)	Rate Constants, $Li(3^2P)$ Product, Measurements	$Li(3^2D)+Ne,Ar$
88751.	Balucani, N., M. Alagia, L. Cartechini, P. Casavecchia, G.G. Volpi, L.A. Pederson and G.C. Schatz, "Dynamics of the $N(^2D)+D_2$ Reaction from Crossed Beam and Quasiclassical Trajectory Studies," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 2414-2422 (2001).	$N(^2D)+D_2$ Product ND Kinetic Energy Angular Distribution Measurements Theory
(89060)	P.E. Surfaces, Interpolated Construction Method	$N(^2D)+H_2$
(88986)	Reaction Dynamics, Reactive Quenching, Branching Channels, Rate Constants, Calculations	$N(^2D)+O_2$
(88698)	Predissociation, (B-X)(2+1) REMPI Spectra, Rydberg State Constants	NH_3 ,ND_3(B)
88752.	Sivakumaran, V., K.P. Subramanian and V. Kumar, "Lifetime Measurement of NO_2 at 423-462 nm," *J. Quant. Spectrosc. Radiat. Transfer* 69, 513-518 (2001).	NO_2* Lifetimes Fluorescence Decays
88753.	Sivakumaran, V., K.P. Subramanian and V. Kumar, "Lifetime Measurements of NO_2 in the Predissociation Region 399-416 nm," *J. Quant. Spectrosc. Radiat. Transfer* 69, 519-524 (2001).	NO_2* Lifetimes Fluorescence Decay Rates Predissociation
88754.	Sivakumaran, V., K.P. Subramanian and V. Kumar, "Self-Quenching and Zero-Pressure Lifetime Studies of NO_2 at 465-490, 423-462 and 399-416 nm," *J. Quant. Spectrosc. Radiat. Transfer* 69, 525-534 (2001).	NO_2* Self-Quenching Lifetimes Fluorescence Decay Rates
88755.	Fantoni, R., M. Giorgi, L. De Dominicis and D.N. Kozlov, "Collisional Relaxation and Internal Energy Redistribution in NO_2 Investigated by Means of Laser Induced Thermal Grating Technique," *Chem. Phys. Lett.* 332, 375-380 (2000).	$NO_2(^2B_1)+M$ Relaxation Thermal Grating Monitor $M=CO_2$,N_2 ,Ar

88756.	Dobson, C.C., and C.C. Sung, "Laser Induced Optical Pumping Measurements of Cross Sections for Fine- and Hyperfine-Structure Transitions in Sodium Induced by Collisions with Helium and Argon Atoms," *Phys. Rev. A: At. Mol. Opt. Phys.* 59, 3402-3407 (1999).	$Na(^2P_{1/2}/^2P_{3/2})$ Fine,Hyperfine Mixing Cross Sections He,Ar Colliders
88757.	Griffin, J., D.R. Worsnop, R.C. Brown, C.E. Kolb and D.R. Herschbach, "Chemical Kinetics of the $NaO(A^2\Sigma^+)+O(^3P)$ Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1643-1648 (2001).	$NaO(A)+O$ $Na+O_2+He$ Rate Constants $Na(^2P)$ Product Branching Ratio
(89118)	Rotational Energy Transfer, Probabilities, Calculations	$Na_2(A,J)+H_2$
(88708)	LIF Spectrum, Lifetime, Rotational Constants, Ground State Assignment	$NiF(^2\Pi_{3/2})$
88758.	Alagia, M., N. Balucani, L. Cartechini, P. Casavecchia, M. van Beek, G.G. Volpi, L. Bonnet and J.C. Rayez, "Crossed Beam Studies of the $O(^3P,^1D)+CH_3I$ Reactions: Direct Evidence of Intersystem Crossing," *Faraday Discuss. Chem. Soc.* 113, 133-150 (1999).	$O(^1D,^3P)+CH_3I$ Crossed Beams IO Product Distributions
88759.	Strekowski, R.S., J.M. Nicovich and P.H. Wine, "Quenching of $O(^1D_2)$ by Cl_2CO: Kinetics and $O(^3P_J)$ Yield," *Chem. Phys. Lett.* 330, 354-360 (2000).	$O(^1D)+COCl_2$ Quenching Rate Constant $O(^3P)$ Yield
(88988)	Reaction Dynamics, Cross Sections, Branching Ratios, Product Energies, Calculations	$O(^1D)+HD$
(88989)	Reaction Dynamics, Probabilities, Angula Momenta Effects, Calculations	$O(^1D)+H_2$
(88990)	Reaction Dynamics, Rate Constants, Insertion Role, Calculations	$O(^1D)+H_2$
88760.	Estupinan, E.G., R.E. Stickel and P.H. Wine, "An Investigation of N_2O Production from Quenching of $OH(A^2\Sigma^+)$ by N_2," *Chem. Phys. Lett.* 336, 109-117 (2001).	$OH(A)+N_2$ Quenching N_2O Product Quantum Yield
88761.	Miller, H.C., J.E. McCord, J. Choy and G.D. Hager, "Measurement of the Radiative Lifetime of $O_2(a^1\Delta_g)$ Using Cavity Ringdown Spectroscopy," *J. Quant. Spectrosc. Radiat. Transfer* 69, 305-325 (2001).	$O_2(a),v=0$ Radiative Lifetime Measurement
(88714)	Vibrational Lifetimes, Spectral Constants, Electronic Energy, Calculations	PF(a)
(88995)	Reaction Dynamics, Cross Sections, Product Energies, Branching Ratios, Calculations	$S(^1D)+H_2,HD,D_2$
(88721)	Predissociation, (C-X) Cavity Ringdown Absorption, F.C. Factors	$S_2O(C,v\geq 4)$
(89066)	Lifetime, P.E. Curves, Low-lying States, Spectral Constants, Calculations	SiP(B)

88762. Redondo, C., M.N.S. Rayo, J.A. Fernandez, D. Husain and F. Castano, "Collisionally Induced Intramultiplet Mixing of $Sr(5^3P_J)$ Metastable States by Ne, Kr and Xe Atoms," *Chem. Phys. Lett.* 331, 365-372 (2000).

$Sr(5^3P_J)+Rg$
Mixing
Rate Constants
Measurements

88763. Redondo, C., M.N.S. Rayo, J.A. Fernandez, D. Husain and F. Castano, "Collisionally Induced Intramultiplet Mixing of $Sr(5^3P_J)$ Metastable States by He, Ar and Sr Ground State Atoms," *Chem. Phys.* 264, 123-134 (2001).

$Sr(5^3P_J)+M$
Mixing
Rate Constants
M=He,Ar,Sr
LIF
Measurements

88764. Biemont, E., J. Lidberg, S. Mannervik, L.-O. Norlin, P. Royen, A. Schmitt, W. Shi and X. Tordoir, "Lifetimes of Metastable States in Sr^+," *Eur. Phys. J. D* 11, 355-365 (2000).

$Sr^+(^2D_{5/2,3/2})$
Metastable
Lifetimes
Measurements
Calculations

28. FRANCK-CONDON FACTORS/TRANSITION PROBABILITIES

(See also Section 27 for Lifetimes and Transition Probabilities)

88765. Bouanich, J.-P., "Comment on the Paper 'Electric Dipole Moment Function of $^{12}C^{16}O$' by Kiriyama and Rao," *J. Quant. Spectrosc. Radiat. Transfer* 69, 1 (2001).

CO
Electric Dipole
Moment Function
Erratum

(89047) F.C. Factors, P.E. Curves, Transitions, Spectral Constants, Calculations

CdRg(B,A-X)

88766. Staszewska, G., "Transition Moments between $w^3\Pi_g$ State and the First Three $^3\Sigma_u$ and $^3\Pi_u$ States of the Hydrogen Molecule," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 2308-2311 (2001).

H_2(w-k,d,c)
H_2(w-f,e,b)
Dipole
Transition Moments
w-State Constants
Calculations

88767. Merawa, M., D. Begue, M. Rerat and C. Pouchan, "Long-Range Dispersion Coefficients for the Low-lying Electronic States of Mg_2 from the Calculation of the Frequency-Dependent Dipole Polarizabilities of Mg in Its Ground and Excited States," *Chem. Phys. Lett.* 334, 403-410 (2001).

Mg_2
Low-lying States
Oscillator
Strengths
Calculations

88768. Mar, S., C. Perez, V.R. Gonzalez, M.A. Gigosos, J.A. del Val, I. de la Rosa and J.A. Aparicio, "Experimental Transition Probabilities in N^+ Lines," *Astron. Astrophys., Suppl. Ser.* 144, 509-515 (2000).

N^+
108 Transition
Probabilities
Visible Region

88769. Di Stefano, G., and A. Ricci, "Strength of the $NF(b^1\Sigma^+ \rightarrow X^3\Sigma^-)$ Transition. II. Estimate of the NF Ground State Dissociation Limit by Analysis of the $\Delta v=0$ Emission Sequence," *Chem. Phys. Lett.* 331, 196-202 (2000).

NF(b-X)
Emission Intensities
F.C. Factors
b(v) Distributions

88770. Gamache, R.R., and A. Goldman, "Einstein A-Coefficient, Integrated Band Intensity, and Population Factors: Application to the ($a^1\Delta_g$-$X^3\Sigma_g^-$), (0,0) O_2 Band," *J. Quant. Spectrosc. Radiat. Transfer* 69, 389-401 (2001).

O_2(a-X),(0,0)
Transition
Probability
Band Intensity
Evaluation

(89065) Transition Moment, P.E. Curves, Low-lying States, Avoided Crossings

O_2(f-X)

(88711) Photoionization Spectra, Non-F.C. Factors, Branching Ratios

O_2^+/O_2

88771. Alonso-Medina, A., C. Colon and C. Herran-Martinez, "Experimentally Determined Transition Probabilities for Lines of Pb and the 220.35 nm Line of Pb^+," *J. Quant. Spectrosc. Radiat. Transfer* 68, 351-362 (2001).

Pb,Pb^+
Transition
Probabilities
Measurements

88772. Lee, S., H. Sun, B. Kim and K.F. Freed, "Quantum Interference and Asymptotic Interactions in the Photodissociation of SH: Total Cross Section and Branching Ratios," *J. Chem. Phys.* 114, 5537-5544 (2001).

SH($2^2\Pi$,$^2\Delta$,$^2\Sigma^-$,A-X)
Transition
Dipole Moments
Photodissociation
Dynamics
Potential Control

(88721) F.C. Factors, Cavity Ringdown Absorption, $\nu_2' \geq 4$ Predissociation

S_2O(C-X)

88773. Alonso-Medina, A., and C. Colon, "Interpretation of the Spectrum of Sn^+: Experimental and Theoretical Transition Probabilities," *Phys. Scr.* 61, 646-651 (2000).

Sn^+
36 Lines
Transition
Probabilities

88774. Bowers, C.J., D. Budker, S.J. Freedman, G. Gwinner, J.E. Stalnaker and D. DeMille, "Experimental Investigation of the ($6s^2\ ^1S_0 \rightarrow 5d6s\ ^3D_{1/2}$) Forbidden Transitions in Atomic Ytterbium," *Phys. Rev. A: At. Mol. Opt. Phys.* 59, 3513-3526 (1999).

Yb($^3D_{1/2}$-$^1S_0$)
Forbidden
Transition
Probability

29. LINESHAPES/STRENGTHS

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CHF_3
Broadening
Coefficients
CCl_4,CH_4,Rg
Colliders

88776. Korek, M., "Non-Integral Expression for the Relative Intensities in the Pure Rotational Infrared Transitions of a Diatomic Molecule," *J. Quant. Spectrosc. Radiat. Transfer* 67, 323-326 (2000).

Rotational IR
Line Intensities
Diatomics
CO
Analysis Method

88777. Di Rosa, M.D., and R.L. Farrow, "Temperature-Dependent Collisional Broadening and Shift of Q-Branch Transitions in the ($B \leftarrow X$),(0,0) Band of CO Perturbed by N_2, CO_2 and CO," *J. Quant. Spectrosc. Radiat. Transfer* 68, 363-375 (2001).

CO(B-X),(0,0)
Collisional
Broadening
Q-Branch

CO, CO_2, N_2
Colliders

88778. Vereschagin, K.A., V.V. Smirnov, E.T.H. Chrysostom and J.W. Nibler, "High-Resonance CARS Study of Collisional Broadening of the ν_2 Q-Branch of Acetylene," *J. Raman Spectrosc.* 31, 719-723 (2000).
C_2H_2, ν_2
Line Broadening
CARS Monitor
Q-Branch

88779. Mandin, J.-Y., V. Dana and C. Claveau, "Line Intensities in the ν_5 Band of Acetylene $^{12}C_2H_2$," *J. Quant. Spectrosc. Radiat. Transfer* 67, 429-446 (2000).
C_2H_2, ν_5
Line Intensities
FT Spectral
Measurements

88780. Lange, K.R., N.P. Wells, K.S. Plegge and J.A. Phillips, "Integrated Intensities of O-H Stretching Bands: Fundamentals and Overtones in Vapor Phase Alcohols and Acids," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3481-3486 (2001).
$ROH(C_1\text{-}C_4)$
CF_3CH_2OH
CH_3COOH
HNO_3
$(1\text{-}4)\nu_{OH}$
Vibrational
Band Intensities
Measurements

(88676) IR, Raman Intensities, Measurements
C_4H_7F

88781. Claveau, C., A. Henry, D. Hurtmans and A. Valentin, "Narrowing and Broadening Parameters of H_2O Lines Perturbed by He, Ne, Ar, Kr and Nitrogen in the Spectral Range 1850-2140 cm^{-1}," *J. Quant. Spectrosc. Radiat. Transfer* 68, 273-298 (2001).
H_2O
1850-2140 cm^{-1}
Broadening
Coefficients
N_2, Rare Gases

88782. Kissel, A., H.-D. Kronfeldt, B. Sumpf, Yu.N. Ponomarev and B.A. Tikhomirov, "Line Broadening and Life Shift of H_2S Absorption Lines in the ν_2 Band: Collisions with H_2O and Ar in a Three Component Mixture," *J. Quant. Spectrosc. Radiat. Transfer* 69, 573-583 (2001).
H_2S, ν_2
Line Broadening
Coefficients
Ar, H_2 Colliders

(88750) Lineshapes, Lifetime, Imprisonment Cell, Measurements
$Kr(^3P_1\text{-}^1S_0)$

(89089) Infrared Intensities, Isomers, Structural Calculations, Geometries, Frequencies
Mg^+NO

88783. Dhib, M., J.-P. Bouanich, H. Aroui and A. Picard-Bersellini, "Analysis of N_2, O_2, CO_2 and Air Broadening of Infrared Spectral Lines in the ν_4 Band of NH_3," *J. Quant. Spectrosc. Radiat. Transfer* 68, 163-178 (2001).
NH_3, ν_4
Broadening
Coefficients
Air, CO_2, N_2, O_2
Colliders

88784. Baldacchini, G., F. D'Amato, G. Buffa, O. Tarrini, M. De Rosa and F. Pelagalli, "Temperature Dependence of Foreign Gas Broadening and Shift of the aQ(9,9) Transition Line of Ammonia," *J. Quant. Spectrosc. Radiat. Transfer* 68, 625-633 (2001).
NH_3, aQ(9,9)
Broadening
Coefficients
Air, N_2, H_2
O_2, He, Ar
Colliders

		180-380 K
88785.	Gillis, J.R., A. Goldman, G. Stark and C.P. Rinsland, "Line Parameters for the ($A^2\Sigma^+$-$X^2\Pi$) Bands of OH," *J. Quant. Spectrosc. Radiat. Transfer* 68, 225-230 (2001).	OH(A-X) $v' \leq 3, v'' \leq 2$ Line Positions Intensities 296,4000 K

30. ANALYSIS/MONITORING TECHNIQUES

(See also Section 32 for 2-D Mapping Methods)

88786.	Meigas, K., "Method for Small Particle Detection by Laser," *Opt. Eng.* 37, 2587-2591 (1998).	Small Particles Laser Monitoring Method
(88559)	Atmospheric OH, Liquid Scrubber, Monitor	Chromatography
88787.	Messer, B.M., D.E. Stielstra, C.D. Cappa, K.W. Scholtens and M.J. Elrod, "Computational and Experimental Studies of Chemical Ionization Mass Spectrometric Detection Techniques for Atmospherically Relevant Peroxides," *Int. J. Mass Spectrom. Ion Process.* 197, 219-235 (2000).	Chemical Ionization Mass Analysis CH_3OOH H_2O_2 Monitoring Method
(88482)	$Kr^+(^2P_{1/2,3/2})$, $Xe^+(^2P_{1/2,3/2})$ Spin-Orbit States, Mobility/Mass Analysis Technique	Ion Monitoring Method
88788.	Stuewer, D., and N. Jakubowski, "Elemental Analysis by Inductively Coupled Plasma Mass Spectrometry with Sector Field Instruments: A Progress Report," *J. Mass Spectrom.* 33, 579-590 (1998).	ICP/ Mass Analysis Double Focusing Instruments Review
88789.	Goyette, A.N., J.E. Lawler, L.W. Anderson, D.M. Gruen, T.G. McCauley, D. Zhou and A.R. Krauss, "C_2 Swan Band Emission Intensity as a Function of C_2 Density," *Plasma Sources Sci. Technol.* 7, 149-153 (1998).	C_2(d-a) Emission/ Absorption Comparison Measurements Diamond Formation $Ar/H_2/CH_4$ Conditions
88790.	Welz, B., and M. Sperling, "*Atomic Absorption Spectrometry,*" 3rd Revised Edition, 941 pp., Wiley-VCH, Weinheim, Germany (1999).	Atomic Absorption Analysis Handbook
88791.	Booth, J.-P., G. Cunge, F. Neuilly and N. Sadeghi, "Absolute Radical Densities in Etching Plasmas Determined by Broad-Band Ultraviolet Absorption Spectroscopy," *Plasma Sources Sci. Technol.* 7, 423-430 (1998).	UV Absorption AlF, CF, CF_2 S_2, SiF_2

(88533)	Hydrocarbon Small I.C. Engine Emissions, Speciation, Measurements	Absorption FTIR
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88793.	Fukuchi, T., T. Fujii, N. Goto, K. Nemoto and N. Takeuchi, "Evaluation of Differential Absorption Lidar Measurement Error by Simultaneous DIAL and Null Profiling," *Opt. Eng.* 40, 392-397 (2001).	Absorption DIAL O_3 Troposphere 2 Laser Background Correction
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31. FLAME CONCENTRATION MEASUREMENTS

(See also Section 34 for Flame Species Profiles)

(88423) Natural Gas/Air, 2-Stage Flames, Measurements, Modeling — Species Concentrations

32. MAPPING/TOMOGRAPHIC METHODS

(88380) Planar Laser Imaging Method — Dense Sprays

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		Plasmas Monitoring
(89013)	2-D Velocity Mapping, Laser Ablation, Measurements	B
(88859)	Product Velocity Map Imaging, ^{13}CO 2-Photon Dissociation, (1+1) REMPI	$C(^1D)$
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(88871)	Product Angular Distributions, Velocity Mapping, MPD/MPI C_6H_5I, Dynamics	I-Atom
88809.	Wang, L., H. Kohguchi and T. Suzuki, "Femtosecond Time-Resolved Photoelectron Imaging," *Faraday Discuss. Chem. Soc.* 113, 37-46 (1999).	fs Imaging Method NO 2-Color Photoionization Dynamics Probe
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88812.	Lian, Y.S., and K. Xu, "A Gas Kinetic Scheme for Multimaterial Flows and Its Application in Chemical Reactions," *J. Computat. Phys.* 163, 349-375 (2000).	Kinetic Modeling Reactive Flows Multicomponent
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(88588)	Kinetic Modeling, NO Formation, Reduced Schemes, Adequacies	CH_4/Air
(88498)	Organophosphates, Inhibition, Species Profiles, Kinetic Modeling	$CH_4/P/O_2$/Ar $H_2/P/O_2$/Ar
88814.	Saastamoinen, J.J., P.T. Kilpinen and T.N. Norstrom, "New Simplified Rate Equation for Gas Phase CO Oxidation at Combustion," *Energy Fuels* 14, 1156-1160 (2000).	Kinetic Modeling CO/O_2 Moist Air New Simplified Mechanism 1000-1700 K
88815.	Varatharajan, B., and F.A. Williams, "Chemical Kinetic Descriptions of High Temperature Ignition and Detonation of Acetylene/Oxygen/Diluent Systems," *Combust. Flame* 124, 624-645 (2001).	Kinetic Modeling C_2H_2/O_2/Diluent Ignition Detonation Full/Reduced Schemes
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88817.	Liakos, H.H., M.A. Founti and N.C. Markatos, "The Effect of Pressure in Industrial Propane/Oxygen Flames," *Int. J. Energy Res.* 25, 17-28 (2001).	Kinetic Modeling C_3H_8/O_2 Turbulent Flows Pressure Effects

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Kinetic Modeling
$CH_2(OCH_3)_2/O_2$
Product Profiles
Jet-Stirred Reactor
Mechanisms

(88618) NO Control, Reburn Kinetics, Jet Stirred Reactor, Kinetic Modeling — n-$C_4H_{10}/NO/O_2$

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Kinetic Modeling
n-$C_{16}H_{34}/O_2$
Jet Stirred Reactor
Product Profiles
Mechanism

88820. Hughes, K.J., A.S. Tomlin, E. Hampartsoumian, W. Nimmo, I.G. Zsely, M. Ujvari, T. Turanyi, A.R. Clague and M.J. Pilling, "An Investigation of Important Gas Phase Reactions of Nitrogenous Species from the Simulation of Experimental Measurements in Combustion Systems," *Combust. Flame* 124, 573-589 (2001).
Nitrogen
Combustion
Kinetics
Sensitivity
Analysis
Modeling/Experiment
Comparisons
Discrepancies

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(see also Section 4 for Coal Pyrolysis)

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Pyrolysis
C_2H_3Br
Rate Constant
Major Products

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Pyrolysis
$ClCH_2CH(R)O$
$HOCH_2CH(CF_3)O$
$R=H,CH_3,CF_3$
Dissociation
Rate Constants
Energy Barriers
Channels

88823. Lifshitz, A., A. Suslensky and C. Tamburu, "Thermal Decomposition of 4-Methylpyrimidine: Experimental Results and Kinetic Modeling," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3542-3554 (2001).
Pyrolysis
$(CH_3)C_4H_3N_2$
Rate Constant
Products
Shock Tube
Mechanism

(89002) Pyrolysis, c-C_5H_5 Source, Dimerization to Naphthalene, $C_{10}H_8$ — c-$C_5H_5C(C_6H_5)_3$

36. KINETIC MODELING/SENSITIVITIES/RATE CONSTANTS

(See also Section 15 for Ion Reaction Rate Constants, Section 27 for Excited State Rate Constants, Section 35 for Pyrolysis Rate Constants, Section 39 for Unimolecular Rate Constants, Section 40 for Theoretically Calculated Values and Section 45 for Energy Relaxation Rate Constants)

88824. Ranzi, E., M. Dente, A. Goldaniga, G. Bozzano and T. Faravelli, "Lumping Procedures in Detailed Kinetic Modeling of Gasification, Pyrolysis, Partial Oxidation and Combustion of Hydrocarbon Mixtures," *Prog. Energy Combust. Sci.* 27, 99-139 (2001).

Kinetic Modeling
Pyrolysis
Gasification
Partial Oxidation
Combustion
Reaction Lumping Techniques

88825. Soller, R., J.M. Nicovich and P.H. Wine, "Temperature-Dependent Rate Coefficients for the Reactions of $Br(^2P_{3/2})$, $Cl(^2P_{3/2})$ and $O(^3P_J)$ with $BrONO_2$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1416-1422 (2001).

$BrONO_2+Br,Cl$
$BrONO_2+O$
Rate Constants
T,P Dependences

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$C+C_2D_2$
Crossed Beam
Cross Sections
D Product
Energy Barrier

88827. Chastaing, D., S.D. Le Picard, I.R. Sims, I.W.M. Smith, W.D. Geppert, C. Naulin and M. Costes, "Rate Coefficients and Cross Sections for the Reactions of $C(^3P_J)$ Atoms with Methylacetylene and Allene," *Chem. Phys. Lett.* 331, 170-176 (2000).

$C+C_3H_4$
Rate Constants
T Dependences
Measurements

88828. Wu, F., and R.W. Carr, "Kinetics of CH_2ClO Radical Reactions with O_2 and NO, and the Unimolecular Elimination of HCl," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1423-1432 (2001).

$CH_2ClO+NO,O_2$
$CH_2ClO\rightarrow$
Rate Constants
T,P Dependences

88829. Canosa-Mas, C.E., T.J. Dillon, H. Sidebottom, K.C. Thompson and R.P. Wayne, "A Study of the OH Initiated Oxidation of Chlorinated Ethenes in the Gas Phase," *Phys. Chem. Chem. Phys.* 3, 542-550 (2001).

CH_2Cl_2+Cl
CH_2Cl_2+OH
Rate Constants
P Dependence
Mechanisms

88830. Martinez, E., J. Albaladejo, E. Jiminez, A. Notario and Y. Diaz de Mera, "Temperature Dependence of the Limiting Low- and High Pressure Rate Constants for the CH_3O+NO_2+He Reaction over the 250-390 K Temperature Range," *Chem. Phys. Lett.* 329, 191-199 (2000).

CH_3O+NO_2+He
Rate Constants
P,T Dependence
Fall-off Parameters
Measurements

88831. Faure, A., C. Rist and P. Valiron, "Temperature Dependence for the $CN+NH_3$ Reaction under Interstellar Conditions: Beyond Capture Theories?," *Astron. Astrophys.* 348, 972-977 (1999).

$CN+NH_3$
Rate Constants
25-300 K
Rotational Effects
Calculations

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C_2H+CH_4
Rate Constants
T Dependence
Measurements
Theory

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C_2H+O_2
Rate Constants
Measurements

88834. Yamada, T., T.D. Fang, P.H. Taylor and R.J. Berry, "Erratum - Kinetics and Thermochemistry of the OH Radical Reaction with CF_3CCl_2H and CF_3CFClH [*J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 5013-5022 (2000)]," *ibid.* 105, 3940 (2001).

CF_3CHCl_2+OH
$CF_3CHFCl+OH$
Rate Constants
Calculations
Erratum

88835. Wilson, Jr., E.W., A.A. Sawyer and H.A. Sawyer, "Rates of Reaction for Cyclopropane and Difluoromethoxydifluoromethane with Hydroxyl Radicals," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1445-1448 (2001).

$(CHF_2)_2O+OH$
c-C_3H_6+OH
Rate Constants
T Dependence

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C_2H_5F+O
$C_2H_4F_2+O$
Rate Constants
T Dependences

88837. Vasvari, G., I. Szilagyi, A.. Bencsura, S. Dobe, T. Berces, E. Henon, S. Canneaux and F. Bohr, "Reaction and Complex Formation between OH Radical and Acetone," *Phys. Chem. Chem. Phys.* 3, 551-555 (2001).

$(CH_3)_2CO+OH$
Rate Constants
Branching Ratio
Measurements
Mechanism

88838. Orlando, J.J., G.S. Tyndall and N. Ceazan, "Rate Coefficients Product Yields from Reaction of OH with 1-Penten-3-ol, (Z)-2-Penten-1-ol, and Allyl Alcohol (2-Propen-1-ol)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3564-3569 (2001).

C_3H_5OH+OH
C_5H_9OH+OH
Rate Constants
Products,Yields

88839. Tranter, R.S., and R.W. Walker, "Rate Constants for H and OH Attack on Propanone, Butanone and Pentan-3-one at 753 K, and the Oxidation Chemistry of the Radicals Formed," *Phys. Chem. Chem. Phys.* 3, 1262-1270 (2001).

$RCOR'+H,OH$
Rate Constants
C_3-C_5 Ketones
Measurements

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$C_2H_5CH(O)CH_3 + NO$
$C_2H_5CH(O)CH_3 + O_2$
Rate Constants
T,P Dependences

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$C_4H_8 + O_3$
Rate Constants
T,P Dependences
Measurements

88842. Lewin, A.G., D. Johnson, D.W. Price and G. Marston, "Aspects of the Kinetics and Mechanism of the Gas Phase Reactions of Ozone with Conjugated Dienes," *Phys. Chem. Chem. Phys.* 3, 1253-1261 (2001).

Dienes + O_3
Rate Constants
6 C_5-C_8 Dienes
OH Product Yields
Measurements

88843. Berho, F., and R. Lesclaux, "Gas Phase Reactivity of the Cyclohexadienyl Radical with O_2 and NO and Thermochemistry of the Association Reaction with NO," *Phys. Chem. Chem. Phys.* 3, 970-979 (2001).

c-$C_6H_7 + NO$
c-$C_6H_7 + O_2$
Rate Constants
Measurements
Thermochemistry

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$Ca + O_2 + N_2$
Rate Constants
Fall-off Parameters

88845. Boone, G.D., F. Agyin, D.J. Robichaud, F.-M. Tao and S.A. Hewitt, "Rate Constants for the Reactions of Chlorine Atoms with Deuterated Methanes: Experiment and Theory," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1456-1464 (2001).

$Cl + CH_nD_{4-n}$
Rate Constants
Measurements
Calculation
Comparisons

88846. Cotter, E.S.N., N.J. Booth, C.E. Canosa-Mas, D.J. Gray, D.E. Shallcross and R.P. Wayne, "Reactions of Cl Atoms with CH_3I, C_2H_5I, 1-C_3H_7I, 2-C_3H_7I and CF_3I: Kinetics and Atmospheric Relevance," *Phys. Chem. Chem. Phys.* 3, 402-408 (2001).

$Cl + RI$
$Cl + CF_3I$
$R = C_1$-C_3 Alkyl
Rate Constants
P Independent
Measurements

88847. Ullerstam, M., E. Ljungstrom and S. Langer, "Reactions of Acrolein, Crotonaldehyde and Pivalaldehyde with Cl Atoms: Structure-Activity Relationship and Comparison with OH and NO_3 Reactions," *Phys. Chem. Chem. Phys.* 3, 986-992 (2001).

$Cl + C_2H_3CHO$
$Cl + C_3H_5CHO$
$Cl + (CH_3)_3CCHO$
$Cl + C_2H_5CHO, C_4H_8$
$Cl + C_3H_7CHO$
Rate Constants
Structure Effects

(88896) Product HF(v=1,2) Cross Sections, Crossed Jet Scattering

$F + CH_4$

88848. Becerra, R., S.E. Boganov, M.P. Egorov, V.I. Faustov, O.M. Nefedov and R. Walsh, "The Insertion Reaction of Germylene into the Si-H Bond of Silane: Absolute Rate Constants, Temperature Dependence, RRKM Modeling and Quantum Chemical (ab Initio and DFT) Calculations," *Phys. Chem. Chem. Phys.* 3, 184-192 (2001).

$GeH_2 + SiH_4$
Rate Constants
T Dependence
RRKM Modeling
$\Delta H_f(GeH_2)$

88849. Brown, S.S., J.B. Burkholder, R.K. Talukdar and A.R. Ravishankara, "Reaction of Hydroxyl Radical with Nitric Acid: Insights into Its Mechanism," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1605-1614 (2001).

$HNO_3 + OH$
Rate Constants
^{18}O,D-Labeling
T,P Dependences
Measurements
Mechanism

88850. Tomas, A., E. Villenave and R. Lesclaux, "Reactions of the HO_2 Radical with CH_3CHO and $CH_3C(O)O_2$ in the Gas Phase," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3505-3514 (2001).

$HO_2 + CH_3CHO$
$HO_2 + CH_3C(O)O_2$
Rate Constants
$CH_3CH(OH)O_2$
UV Spectrum
Thermochemistry

88851. Herndon, S.C., P.W. Villalta, D.D. Nelson, J.T. Jayne and M.S. Zahniser, "Rate Constant Measurements for the Reaction of HO_2 with O_3 from 200 to 300 K Using a Turbulent Flow Reactor," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1583-1591 (2001).

$H^{18}O_2 + O_3$
Rate Constants
T Dependence

(89109) Reactive/Vibrational Relaxation Channels, Rate Constants, Measurements

$H_2O(v) + H,H_2O$
$OH(v=1) + H,H_2O$

88852. Knight, G.P., and J.N. Crowley, "The Reactions of IO and HO_2, NO and CH_3SCH_3: Flow Tube Studies of Kinetics and Product Formation," *Phys. Chem. Chem. Phys.* 3, 393-401 (2001).

$IO + HO_2$
$IO + NO$
$IO + (CH_3)_2S$
Rate Constants
T Dependences
Channels

88853. Campbell, M.L., "Kinetic Study of Gas Phase $Lu(^2D_{3/2})$ with O_2, N_2O and CO_2," *Chem. Phys. Lett.* 330, 547-550 (2000).

$Lu + CO_2, O_2$
$Lu + N_2O$
Rate Constants
T Dependences

(88820) Nitrogen Combustion Kinetics, Sensitivity Analysis, Modeling/ Experiment Comparisons, Discrepancies

NO_x Kinetics

(88757) Rate Constants, $Na(^2P)$ Product Branching Ratio, Measurements

$Na + O_2 + He$
$NaO(A) + O$

88854. Yujing, M., and A. Mellouki, "Temperature Dependence for the Rate Constants of the Reaction of OH Radicals with Selected Alcohols," *Chem. Phys. Lett.* 333, 63-68 (2001).

$OH + C_3H_7OH$
$OH + C_4H_9OH$
Rate Constants
T Dependences

88855. Becerra, R., J.P. Cannady and R. Walsh, "Silylene Does React with Carbon Monoxide: Some Gas Phase Kinetic and Theoretical Studies," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1897-1903 (2001).
$SiH_2+CO(+SF_6)$
Rate Constants
P,T Dependences
Measurements
RRKM Analysis

37. PHOTOLYSIS/MPD

(See also Section 38 for Photolytic Product Distributions and Section 42 for Laser Control)

88856. Yokoyama, A., K. Yokoyama and T. Takayanagi, "Photodissociation Dynamics of $CBrClF_2$ at 157.6 nm. I. Experimental Study Using Photofragment Translational Spectroscopy," *J. Chem. Phys.* 114, 1617-1623 (2001).
$CBrClF_2+h\nu$
Products
Channels
Branching Ratios
Measurements

88857. Yokoyama, K., A. Yokoyama and T. Takayanagi, "Photodissociation Dynamics of $CBrClF_2$ at 157.6 nm. II. A Theoretical Study Using Wavepacket Propagation," *J. Chem. Phys.* 114, 1624-1630 (2001).
$CBrClF_2+h\nu$
Photodissociation Dynamics
Triple Product Channel
Calculations

(88808) 2-D Ion Imaging, MPI, Mass Analysis, Overview
$CD_3I,DI+h\nu$
$O_2+h\nu$

88858. Amaral, G., K. Xu and J. Zhang, "H-Atom Product Channels in the Photodissociation of CH_3Cl, CH_3Br and CH_3I at 121.6 nm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1115-1120 (2001).
$CH_3Cl+h\nu$
$CH_3Br,CH_3I+h\nu$
H Product Channels
Energies
Mechanisms

(88444) Thermal Explosions, Light Initiated, Theory
$CH_4/Cl_2+h\nu$

88859. Bakker, B.L.G., and D.H. Parker, "Photodissociation Dynamics of $^{13}C^{16}O$ Excited by 193 nm Light," *Chem. Phys. Lett.* 330, 293-299 (2000).
$^{13}CO+2h\nu$
$C(^1D)$ Yield
Spectrum
$D(^{13}CO)$
Mechanism

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MPD
CF_3CHClF
Product Analysis
CF_2, CF_3CF
Roles

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$CH_2BrCOCl+h\nu$
Photodissociation Dynamics

Rate Constants
Branching Ratios
Calculations

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$C_2H_5 + h\nu$(245 nm)
H Product
Energies
Angular
Distributions
2 Channels
Branching Ratio

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IR MPD
C_3F_6/HCl
$CFCF_3$ Formation
$CFCF_3 + HCl$
$CFCF_3$
Isomerization
Relative Rates

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s-$C_3H_3N_3 + h\nu$
HCN(J) Energies
Mechanism
CARS Monitor

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c-$C_3H_3N_3 + h\nu$
P.E. Surface
Dynamics
HCN Product
Energies

88866. Arnold, P.A., B.R. Cosofret, S.M. Dylewski, P.L. Houston and B.K. Carpenter, "Evidence of a Double Surface Crossing between Open- and Closed-Shell Surfaces in the Photodissociation of Cyclopropyl Iodide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1693-1701 (2001).

c-$C_3H_5I + h\nu$
Gas/Solution
C_3H_5 Product
Dynamics

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MPD
$C_3H_6Br_2$
fs Dynamics
Mass Analysis
Mechanism

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$(CH_3)_2CO + h\nu$
Quantum Yields
248,308 nm
H_2O Effects

88869. Zhitneva, G.P., "Multiphoton Infrared Absorption by Allylmethane, Allyltrimethylmethane and Allytrimethylgermane Molecules," *High Energy Chem., Russia* 32, 280-281 (1998).

IR MPD
$CH_3(C_3H_5)$
$(CH_3)_3C(C_3H_5)$
$(CH_3)_3Ge(C_3H_5)$
Collision Free

Energy
Dependences

88870. Arey, J., S.M. Aschmann, E.S.C. Kwok and R. Atkinson, "Alkyl Nitrate, Hydroxyalkyl Nitrate and Hydroxycarbonyl Formation from the NO_x-Air Photooxidations of C_5-C_8 *n*-Alkanes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1020-1027 (2001).

$RH/NO_x/Air + h\nu$
$RH = C_5$-C_8 *n*-Alkanes
Product Yields
$RONO_2$, $R(OH)R'ONO_2$
$RCOR'(OH)R''$
Mechanisms

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MPD/MPI
C_6H_5I
Product Velocity
Mapping
Dynamics

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$C_6H_5CH_3 + h\nu$
266 nm
Photoelectron
Spectrum
$C_6H_5CH_2^+$ Ions

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IR MPD
$(CH_3)_3C(C_3H_5)$
$(CH_3)_3Ge(C_3H_5)$
Average
Absorbed Energies

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$RCOR' + h\nu$
193 nm
Decay Times
Predissociation
Mechanisms

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MPD/MPI
$Cd(CH_3)_2$
Energy Fluence
Dependences
Fragments

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$Cs + Cs + h\nu$
1_u-State
Photoassociation
Cold Cs_2
Formation

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IR MPD
$(CH_3)_3Ge(C_3H_5)$
Laser Fluence
Effects
Efficiencies
Pulse Length

(89022) Laser Control, Excitation Paths, Phase Lags

MPD/MPI
HI,H_2S

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HNCO+hν
Photodissociation
Dynamics
S_1/S_0 Conversion
Bending/Stretch
Roles

88879. Balint-Kurti, G.G., L. Fusti-Molnar and A. Brown, "Photodissociation of HOBr. II. Calculation of Photodissociation Cross Sections and Photofragment Quantum State Distributions for the First Two Ultraviolet Absorption Bands," *Phys. Chem. Chem. Phys.* 3, 702-710 (2001).

HOBr+hν
photodissociation
Absorption
Cross Sections
OH(v,J) Product
Distribution
Calculations

88880. Amaral, G., K. Xu and J. Zhang, "H+NO_2 Channels in the Photodissociation of HONO at 193.3 nm," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1465-1475 (2001).

HONO+hν
H,NO_2 Channel
Product Energies

88881. Roehl, C.M., T.L. Mazely, R.R. Friedl, Y. Li, J.S. Francisco and S.P. Sander, "NO_2 Quantum Yield from the 248 nm Photodissociation of Peroxynitric Acid (HO_2NO_2)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1592-1598 (2001).

HO_2NO_2+hν
NO_2 Product
Quantum Yield
Mechanism

88882. Luong, A.K., T.G. Clements, M.S. Resat and R.E. Continetti, "Energetics and Dissociative Photodetachment Dynamics of Superoxide-Water Clusters: $O_2^-(H_2O)_n$, n=1-6," *J. Chem. Phys.* 114, 3449-3455 (2001).

$O_2^-H_2O)_{n=1\text{-}6}$+hν
Hydration
Energies
Mechanisms

88883. Bahou, M., L. Schriver-Mazzuoli and A. Schriver, "Infrared Spectroscopy and Photochemistry at 266 nm of the Ozone Dimer Trapped in an Argon Matrix," *J. Chem. Phys.* 114, 4045-4052 (2001).

$(O_3)_2$+hν
Trapped
Matrix Study
Pathways

(88772) Photodissociation Dynamics, ($2^2\Pi,^2\Delta,^2\Sigma^-$,A-X) Transition Dipole Moments, Calculations

SH+hν

88884. Laptev, V.B., L.M. Tumanova and E.A. Ryabov, "Selective Dissociation of $Si(OCH_3)_4$ and $[(CH_3)_3Si]_2O$ Molecules by the Action of a Pulsed CO_2 Laser," *High Energy Chem., Russia* 32, 108-113 (1998).

IR MPD
$Si(OCH_3)_4$
$((CH_3)_3Si)_2O$
Main Products

		Isotopic Selectivity
88885.	Zhitneva, G.P., "Infrared Multiphoton Dissociation of Allyltrimethylstannane in Collisionless and Collisional Modes," *High Energy Chem., Russia* 31, 275-280 (1997).	IR MPD $(CH_3)_3Sn(C_3H_5)$ Fragments Mechanism

38. REACTION PRODUCT-ENERGY DISTRIBUTIONS

(See also Section 37 for Product Distributions and Section 40 for Theoretically Calculated Reaction Product Distributions)

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88887.	Chen, K.-m., "Angular Momentum Coupling in Triatomic Predissociations," *Chem. Phys. Lett.* 333, 119-125 (2001).	Triatomic Predissociations Fragment Distributions Theory
(88906)	Triatomic Unimolecular Dissociation, Theory	Product State Distributions
(88737)	Product Rotational Distributions, $Br_2(B).He$ Predissociation, Lifetimes, Modeling	$Br_2(J)$
88888.	Martinez-Haya, B., P. Quintana, L. Banares, P. Samartzis, D.J. Smith and T.N. Kitsopoulos, "The Photodissociation of CH_3SCH_3 and CD_3SCD_3 at 220-231 nm Investigated by Velocity Map Ion Imaging," *J. Chem. Phys.* 114, 4450-4456 (2001).	CH_3 ,CD_3 Kinetic Energy Recoil Angles $(CH_3)_2S,(CD_3)_2S+h\nu$ Anisotropies
88889.	Li, R., W.S. McGivern and S.W. North, "Temperature Dependent Photodissociation Dynamics of ICN at 262 nm," *Chem. Phys. Lett.* 334, 47-54 (2001).	$CN,I(^2P_{1/2,3/2})$ Product Energies $ICN+h\nu$ Scalar/Vector Correlations

88890.	Cheng, Y., J. Han, X. Chen, Y. Ishikawa and B.R. Weiner, "Dynamics of the $O(^3P)+CS_2(X^1\Sigma_g^+)\rightarrow SO(X^3\Sigma^-)+CS(X^1\Sigma^+)$ Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3693-3700 (2001).	CS(v,J),SO(v,J) Product Energy Distributions $O+CS_2$ Measurements
(88913)	Product Energies, C_2H_5CO Unimolecular Dissociation, Trajectory Calculations	C_2H_5 ,CO
88891.	Kim, Z.H., A.J. Alexander, S.A. Kandel, T.P. Rakitzis and R.N. Zare, "Orientation as a Probe of Photodissociation Dynamics," *Faraday Discuss. Chem. Soc.* 113, 27-36 (1999).	$Cl(^2P_{1/2})$ Product Orientation $Cl_2+h\nu$ Polarized Light
88892.	Mueller, J.A., B.F. Parsons, L.J. Butler, F. Qi, O. Sorkhabi and A.G. Suits, "Competing Isomeric Product Channels in the 193 nm Photodissociation of 2-Chloropropene and in the Unimolecular Dissociation of the 2-Propenyl Radical," *J. Chem. Phys.* 114, 4505-4521 (2001).	Cl,HCl Product Energies $C_3H_5Cl+h\nu$ $C_3H_5\rightarrow$ Channels Branching
88893.	Cook, P.A., S.R. Langford, R.N. Dixon and M.N.R. Ashfold, "An Experimental and ab Initio Reinvestigation of the Lyman-α Photodissociation of H_2S and D_2S," *J. Chem. Phys.* 114, 1672-1684 (2001).	H,D,SH(A),SD(A) Product Energies $H_2S,D_2S+h\nu$ 121.6 nm Channels $D_0(D_2S)$
(88911)	Product Distribution, $C_2H_3Br(v)$ Unimolecular Dissociation, P.E. Surface, Branching Ratios, Rate Constants	HBr(v)
88894.	Rudic, S., D. Ascenzi and A.J. Orr-Ewing, "Rotational Distribution of the HCl Products from the Reaction of $Cl(^2P)$ Atoms with Methanol," *Chem. Phys. Lett.* 332, 487-495 (2000).	HCl(v=0,J) Product Distribution $Cl+CH_3OH$ Measurements
88895.	Bean, B.D., F. Fernandez-Alonso and R.N. Zare, "Distribution of Rovibrational Product States for the 'Prompt' Reaction $H+D_2(v=0,j=0\text{-}4)\rightarrow HD(v'=1,2,j')+D$ Near 1.6 eV Collision Energy," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 2228-2233 (2001).	HD(v=1,2,J) Product Energies $H+D_2(v=0,J=0\text{-}4)$ 1.6 eV Collision Energy Measurements Theory
88896.	Harper, W.W., S.A. Nizkorodov and D.J. Nesbitt, "Differential Scattering Dynamics of $F+CH_4\rightarrow HF(v,J)+CH_3$ via High Resolution Infrared Laser Dopplerimetry," *Chem. Phys. Lett.* 335, 381-387 (2001).	HF(v,J) Product Energies $F+CH_4$ Crossed Jet Scattering

88897. Nizkorodov, S.A., W.W. Harper and D.J. Nesbitt, "State-to-State Reaction Dynamics in Crossed Supersonic Jets: Threshold Evidence for Nonadiabatic Channels in $F+H_2$," *Faraday Discuss. Chem. Soc.* 113, 107-117 (1999).

HF(v=3,J)
Product
F+*n*-H_2
Cross Sections
$F(^2P_{1/2})$ Role
Crossed Beams
IR Laser Doppler

88898. Marcy, T.P., J.P. Reid, C.X.W. Qian and S.R. Leone, "Addition-Insertion-Elimination Reactions of $O(^3P)$ with Halogenated Iodoalkanes Producing HF(v) and HCl(v)," *J. Chem. Phys.* 114, 2251-2258 (2001).

HF(v),HCl(v)
Product Energies
CF_3CH_2I+O
CF_2ICF_2H+O
CH_2ClCH_2I+O
Measurements
Mechanisms

88899. Wrede, E., S. Laubach, S. Schulenburg, A. Brown, E.R. Wouters, A.J. Orr-Ewing and M.N.R. Ashfold, "Continuum State Spectroscopy: A High Resolution Ion Imaging Study of IBr Photolysis in the Wavelength Range 440-685 nm," *J. Chem. Phys.* 114, 2629-2646 (2001).

$I,Br(^2P_{1/2,3/2})$
Velocity Mapping
IBr+hν
Dynamics

(89020) Product Variations, Laser Control, CH_3I+hν, IBr+hν, Theory

I/I*;Br/Br*

(88758) Product Distributions, $O(^1D,^3P)+CH_3I$, Crossed Beams

IO

88900. Loesch, H., and J. Moller, "Steric Effects and Vector Correlation in Reactions of K Atoms with Brute Force Oriented Aromatic Molecules," *Faraday Discuss. Chem. Soc.* 113, 241-260 (1999).

KI,R
Product
Angular
Distributions
Orientated
K+RI
Crossed Beams
$RI=C_6H_5I$,
$(CH_3)C_6H_4I$

(88751) Product Translational Energy, Angular Distributions, $N(^2D)+D_2$, Measurements, Theory

ND

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NO(J)
Rotational
Alignment
ClNO+hν
Measurements

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NO(v,J)
Product
Distributions
$N+O_2$
Calculations

88903. Li, Q., R.T. Carter and J.R. Huber, "The Photodissociation Dynamics of Nitric Acid Studied at 193 nm by LIF and REMPI-TOF Methods," *Chem. Phys.*

O,OH(T,J)
Product Energy

Lett. 334, 39-46 (2001). | Distributions $HNO_3 + h\nu$ Channels

88904. Ahmed, M., E.R. Wouters, D.S. Peterka, O.S. Vasyutinskii and A.G. Suits, "Atomic Orbital Alignment and Coherence in N_2O Photodissociation at 193.3 nm," *Faraday Discuss. Chem. Soc.* 113, 425-436 (1999). | $O(^1D_2)$ Alignment Angular Distribution $N_2O + h\nu$

88905. Han, J., X. Chen and B.R. Weiner, "Reaction Dynamics of $O(^3P) + H_2(v=1)$," *Chem. Phys. Lett.* 332, 243-250 (2000). | OH(X,v=0,1) Product Energies $O + H_2(v=1)$ Measurements

39. UNIMOLECULAR PROCESSES

(See also Section 36 for Unimolecular Rate Constants and Section 40 for Reaction Dynamics)

88906. Larregaray, P., L. Bonnet and J.C. Rayez, "On Product State Distributions in Triatomic Unimolecular Reactions: Beyond Phase Space Theory and the Adiabatic Assumption," *J. Chem. Phys.* 114, 3349-3364 (2001). | Unimolecular Dissociation Triatomics Product State Distributions Theory

88907. Jain, S.K., C. Rout and R.C. Rastogi, "Density Functional Study of the Isomerization of MOH, M=Be and Mg," *Chem. Phys. Lett.* 331, 547-552 (2000). | Isomerization BeOH/HBeO MgOH/HMgO Geometries Frequencies Energies

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88909. Owrutsky, J.C., H.H. Nelson and A.P. Baronavski, "Methylsulfonyl Radical Unimolecular Dissociation Studied by Deep-Ultraviolet Ultrafast Photoionization Spectroscopy," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1440-1444 (2001). | Unimolecular Dissociation CH_3SO_2 fs Photoionization Monitor

(88863) Isomerization, IR MPD, C_3F_6/HCl | $CFCF_3/C_2F_4$

88910. Koch, D.M., N.H. Khieu and G.H. Peslherbe, "Ab Initio Studies of the Glyoxal Unimolecular Dissociation Pathways," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3598-3604 (2001). | Unimolecular Dissociation $(CHO)_2$ Channels

		P.E. Surface Calculations
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88912.	Martinez-Nunez, E., and S.A. Vazquez, "Three-Center vs Four-Center HF Elimination from Vinyl Fluoride: A Direct Dynamics Study," *Chem. Phys. Lett.* 332, 583-590 (2000).	Unimolecular Dissociation C_2H_3F HF Elimination Channels Calculations
88913.	Martinez-Nunez, E., A. Pena-Gallego and S.A. Vazquez, "The Unimolecular Dissociation of the Propionyl Radical: A Classical Dynamics Study," *J. Chem. Phys.* 114, 3546-3553 (2001).	Unimolecular Dissociation C_2H_5CO Product Energies Trajectory Calculations
88914.	Burgin, M.O., G.L. Heard, J.M. Martell and B.E. Holmes, "Unimolecular Reaction Kinetics of $CF_2ClCF_2CH_3$ and $CF_2ClCF_2CD_3$: Experimental Evidence for a Novel 1,2-FCl Rearrangement Pathway," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1615-1621 (2001).	Unimolecular Dissociation $CF_2ClCF_2CH_3$ $CF_2ClCF_2CD_3$ Rate Constants Products Branching Ratios
88915.	Heard, G.L., and B.E. Holmes, "1,2-FCl Rearrangement as an Intermediate Step in the Unimolecular 1,3-HCl Elimination from Chlorofluoropropanes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1622-1625 (2001).	Unimolecular Dissociation $CF_2ClCF_2CH_3$ $CF_2ClCF_2CD_3$ HCl,DCl Elimination Mechanism
(88467)	Isomeric Ions, Monitoring Method, Rate Constants, Isomerization Energy	$CH_2CHCH_2^+ + M$ $CH_3CCH_2^+ + M$
88916.	Chuchani, G., A. Rotinov, J. Andres, L.R. Domingo and V.S. Safont, "A Combined Experimental and Theoretical Study of the Homogeneous, Unimolecular Decomposition Kinetics of 3-Chloropivalic Acid in the Gas Phase," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1869-1875 (2001).	Unimolecular Dissociation $(CH_3)_2C(CH_2Cl)COOH$ Rate Constants Measurements Theory
88917.	Lei, W., and R. Zhang, "Theoretical Study of Hydroxyisoprene Alkoxy Radicals and Their Decomposition Pathways," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3808-3815 (2001).	Unimolecular Dissociation C_5H_8OHO

		Isomers Channels
88918.	Chakraborty, D., R.P. Muller, S. Dasgupta and W.A. Goddard III, "Mechanism for Unimolecular Decomposition of HMX (1,3,5,7-Tetranitro-1,3,5,7-tetrazocine), an ab Initio Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1302-1314 (2001).	Unimolecular Dissociation HMX Channels Energies Calculations
(88391)	Unimolecular Dissociation, Channels, Rate Constants, Calculations	α-HMX
88919.	Schmatz, S., P. Botschwina, J. Hauschildt and R. Schinke, "Symmetry Specificity in the Unimolecular Decay of the $Cl^{-}\cdots CH_3Cl$ Complex: Two-Mode Quantum Calculations on a Coupled-Cluster [CCSD(T)] Potential Energy Surface," *J. Chem. Phys.* 114, 5233-5245 (2001).	Unimolecular Decay $Cl^{-}.CH_3Cl$ P.E. Surface Symmetry Specific u,g-State Effects Calculations
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(88475)	Isomerization Dissociation Dynamics, HCO^+ Product Channel	$HOCO^+$
88921.	Walch, S.P., and C.E. Dateo, "Thermal Decomposition Pathways and Rates for Silane, Chlorosilane, Dichlorosilane and Trichlorosilane," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 2015-2022 (2001).	Unimolecular Dissociation SiH_4 ,SiH_3Cl SiH_2Cl_2 ,$SiHCl_3$ Activation Energies Channels Calculations

40. CHEMICAL DYNAMICS - THEORY

(See also Section 37 for Photodissociation Dynamics)

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88923.	Rypkema, H.A., N.M. Donahue and J.G. Anderson, "Near-Field Influence on Barrier Evolution in Symmetric Atom Transfer Reactions: A New Model for Two-State Mixing," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1498-1506 (2001).	Reaction Dynamics Atom Transfer Curve Crossing Model Barrier Dependence
88924.	Donahue, N.M., "Revisiting the Hammond Postulate: The Role of Reactant and Product Ionic States in Regulating Barrier Heights, Locations and Transition State Frequencies," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1489-1497 (2001).	Reaction Dynamics Radical/Molecule Avoided Curve Crossing Analysis
88925.	Wyatt, R.E., C.L. Lopreore and G. Parlant, "Electronic Transitions with Quantum Trajectories," *J. Chem. Phys.* 114, 5113-5116 (2001).	Reaction Dynamics Nonadiabatic Electronic Transitions Wavepacket Method
88926.	Bernshtein, V., and I. Oref, "Dependence of Collision Lifetimes on Translational Energy," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3454-3457 (2001).	Reaction Dynamics A+B AB* Lifetime Collision Energy Dependence
88927.	Althorpe, S.C., "Quantum Wavepacket Method for State-to-State Reactive Cross Sections," *J. Chem. Phys.* 114, 1601-1616 (2001).	Reaction Dynamics A+BC $H+H_2$ State-to-State Cross Sections Wavepacket Method
88928.	Parthiban, S., G. de Oliveira and J.M.L. Martin, "Benchmark ab Initio Energy Profiles for the Gas Phase S_N2 Reactions $Y^-+CH_3X \rightarrow CH_3Y+X^-$ (X,Y=F,Cl,Br): Validation of Hybrid DFT Methods," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 895-904 (2001).	Reaction Dynamics Y^-+CH_3X X/Y Exchange X,Y=F,Cl,Br Energetics
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Energies

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$C+C_2H_4$
P.E. Surfaces
Channels
Energies

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$C+N_2$
$N+CN$
$NCN\rightarrow$
Rate Constants
ΔH_f(CNN,NCN)

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Reaction Dynamics
$CH+N_2$
HNCN Intermediate
Allowed Pathway
Mechanism

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$CH_2FBr,CHFBr_2+OH$
$CHCl_2Br,CHClBr_2+OH$
$CHFClBr+OH$
Rate Constants
T Dependences
Calculations

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CH_2F_2+O
CH_3F+O
CH_4+O
Transition States
Rate Constants
Energies

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Energetics

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$HCHO+OH$
$HCHO+OH^-$
Channels
Energies

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CH_3+HBr
Barrier Height
Rate Constants
T Dependence

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CH_3+H_2
Improved
Tunneling
Algorithm

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CH_3+N
Activation Energy
Reaction Enthalpy

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CH_3F+OH
H-Abstraction
Rate Constants
D-Isotope Effects

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CH_3OCl+O,OH
HCHO,Cl
Major Channel
CH_2OCl Radical
Instability

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CH_4+H
Rate Constants
Barrier Height
Modified
P.E. Surface

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CH_4+OH
Product Energies
Quantum
Scattering Model

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CH_4+OD
$CH_nD_{4-n}+OH$
Rate Constants
T Dependences
Energy Barriers
Calculations

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$C_2(a)+H_2$
Rate Constants
Barrier Height
Data Comparisons

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C_2H+CH_3CCH
Channels
Energies

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C_2H_4+HF
Mechanism
Intermediates

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$C_2H_{6-n}F_n+OH$
$n=2\text{-}5$
Rate Constants
Isomers
Calculations

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C_2H_6+H,O,OH
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H Abstraction
Rate Constants
Barrier Heights
Calculations

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C_2H_6+OH
C_2H_5F,C_2H_5Cl+OH
Rate Constants
New Approach

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$HCCCH_2^++C_2H_2$
$c\text{-}C_3H_3^+$ Product Channel
Mechanism

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$n\text{-}C_5H_{12}+H$
$n\text{-}C_6H_{14}+H$
$H_2(v,J)$ Product
Calculations
Data Comparisons

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$C_6H_5+C_2H_2$
$1\text{-}C_{10}H_7+C_2H_2$
Channels
Rate Constants
Calculations

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C_6H_6+O
Channels
Energies

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$Ca+CO_2$
Channels
Energy Barriers

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$Cd(^1P,^3P,^1S)+GeH_4$
$Hg(^1P,^3P,^1S)+GeH_4$
Pathways
Energetics

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$Cl+CH_4$
Non-Arrhenius Behavior
Assessments

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$Cl+HCN(v)$
$H+HCN(v)$
P.E. Surfaces
Rate Constants
Product CN(v,J)

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Cl+HD
P.E. Surface
van der Waals Interaction
Effects

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Cl+OH
HCl+O
Probabilities
Method
Comparisons

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$Cl+O_3$
$ClO+O$
Channels
Energies

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Cl^-+CH_3Cl
Orientational
Dependences
Model

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Cl^-+CH_3Cl
Cl^-+CH_3Br
Cross Sections
Adequacies

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$Cl^-(H_2O)+CH_3Br$
$Cl^-(H_2O)_2+CH_3Br$
Cluster Effects

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$F^-(H_2O)+CH_3Cl$
Collision Energy
Dependence
Cluster Effects
Channels
Branching Ratios

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$FO,ClO+CH_4$
$BrO+CH_4$
H Abstraction
Rate Constants

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$GeH_2+ROH,(CH_3)_2O$
$SiH_2+ROH,(CH_3)_2O$
P.E. Surfaces
$R=CF_3,CH_3,C_2H_5,H$
Channels
Energies

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$H+D_2(v=J=0)$
Cross Sections
Oscillatory
Structure

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$H+D_2$
Cross Sections
Erratum

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$H+H_2$
Diagonal B.-O. Correction
Probabilities
Effects

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$H+H_2$
Conical Intersecting P.E. Surfaces
Probabilities

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$H+H_2O$
1.43,2.2 eV Energies
Cross Sections
Product Rotational Polarization

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$H+O_2+M$
$Mu+O_2+M$
High Pressure Limit
Rate Constants

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$H^++H_2(v)$
Nonadiabatic Transitions
P.E. Surface

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$HCl+O$
Rate Constants
Tunneling
Energy Barrier

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HNO_3+OH
Transition States
Channels
Energies
Rate Constants
D-Isotope Effects

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HO_2+H
Rate Constants
Non-Arrhenius Behavior

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$HO_4(^2A)$
P.E. Surface
$OH(v=0)+O_3$
Testing

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$H_2(v,J)+H_2(v',J')$
Exchange/ Dissociation Channels
Rate Constants
Calculations

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$H_2O(v)+H$
Rate Constants
Reactive Channels
Calculations

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Li+HF
Probabilities
Product Energies
New Calculation Methods

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$Li(^2P).HF$
Transition State
P.E. Surfaces
Decay Channels
Calculations

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LiH+H
Rate Constants
P.E. Surface
$H_2(v)$ Product

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Jet Flow Conditions
$N+N_2$
State-to-State
Rate Constants
Formulations

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$N+N_2(v)$
Dissociation
Rate Constants

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$N(^2D)+D_2$

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$N(^2D)+O_2$
Reactive Quenching
Branching Channels
Rate Constants

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NO_2+RH,C_6H_6
C_1-C_4 Alkanes
Rate Constants
Energy Barriers
Diesel Ignition
Role

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Reaction Dynamics
$O(^1D)+HD$
Cross Sections
Branching Ratios
Product Energies

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$O(^1D)+H_2$
Probabilities
Angular Momenta
Effects

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$O(^1D)+H_2$
Rate Constants
Insertion
Role

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Reaction Dynamics
$OH+H_2$
New P.E. Surfaces
Rate Constants
Accuracies

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$OH+H_2,D_2$
2 P.E. Surfaces
Comparisons
Evaluations

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Reaction Dynamics
$OH(J)+H_2(J')$
Polarizations
Stereodynamics
Quantum Method

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$PH+H_2O$
Channels
Rate Constants

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$S(^1D)+H_2$,HD,D_2
Cross Sections
Product Energies
Branching Ratios

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$SiCl_4+H$
Rate Constants
Energy Barriers
Calculations
Data Comparisons

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Reaction Dynamics
SiH_3F+H
Rate Constants
Path

41. CHEMICAL KINETICS - GENERAL

(See also Section 21 for Emissions Control Discharge Methods)

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BCl_3/Ar
Discharges
Spectral Emissions
B,B^+,B_2,BO,BCl
Electron Densities

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$Ba \cdots FCH_3$
Intermediate
Pump/Probe
Observations
Lifetime

(89102) V-V Pumping, CO_2 Formation, Mechanism, Measurements — $CO(v)+CO(v')$

(88394) Catalytic Kinetic Oscillations, Coupling Mechanisms — $CO/O_2/Pd$

(88398) Catalytic Oxidation, Discharge Method, Conversion Efficiencies — CO,SO_2

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C_2Cl_4,C_2HCl_3
Destruction
UV,Pulsed Discharge
Efficiencies

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C_2D+CH_3CCH
Crossed Beam
Scattering
Channels
Dynamics

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2 c-C_5H_5/$C_{10}H_8$
Dimerization
c-$C_5H_5C(C_6H_5)_3$
Pyrolysis
Measurements

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Cl_2/Ar,N_2,O_2
Discharges
Dissociation
Efficiencies

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Cl_2/O_2
Discharge
Ions,Neutrals
Product
Modeling

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H_2(v)
Pumping Source
Cs/H_2 Discharge

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NO_2+HO_2
NO_2+OH
Reaction
Intermediates
Channels

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$NO_2+{}^{18}OH$
Intermediates
Branching
Kinetics

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N_2/CH_4
L.P. Discharge
N_2(C,B),CN(B)
Emission Decay
Modeling

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(88710) Transition State Monitoring, $H_3O_2^-$, $D_3O_2^-$ Detachment Spectra — $OH.H_2O$

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(88803) Discharges, SiH(A-X) LIF Measurements — SiH_4/H_2

42. LASERS/INDUCED EFFECTS/MPI

(See also Section 26 for REMPI Spectra)

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Laser Ablation
$Ta,Ta_2O_5/O_2$
TaO_n^+,n=1-4
Product Ions
Mass Analysis

89017. Sankaran, K., K. Sundararajan and K.S. Viswanathan, "Matrix Isolation Infrared Studies of the Reactions of Laser Ablated Uranium with N_2: Reactions beyond Insertion into N_2," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3995-4001 (2001).

Laser Ablation
$U(s)/N_2$
Matrix Study
UN
Product FTIR

89018. Simons, J.P., "Sterochemistry and Control in Molecular Reaction Dynamics," *Faraday Discuss. Chem. Soc.* 113, 1-25 (1999).

Laser Control
Chemical Reactions
Stereodynamics
Overview

(88999) Laser Pump/Probe, Real Time Transition State Observations, Lifetime

$Ba...FCH_3$

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Laser Population
Control
HCHS
Selective
Vibration Level
Pumping

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Laser Control
$CH_3I+h\nu$
$IBr+h\nu$
I/I*;Br/Br*
Product Variations
Theory

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Laser Control
$H+H_2$
Isotopes
Possibilities

(88920) Laser Isomerization Control, Theory

HCN/HNC

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Laser Control
HI,H_2S
MPD/MPI
Excitation Paths
Phase Lags

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Laser Control
IR MPD
H_2^+,HD^+
Vibrational
Trapping
Analysis

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(88859) 2-Photon Dissociation of ^{13}CO, Product Velocity Map Imaging — REMPI,$^{13}C(^1D)$

(88741) (2+1) CO(B) Pumping, CO^+(B-X) LIF, Quenching Rate Constants, Nine Collider Species — REMPI,CO

89026. Schick, C.P., and P.M. Weber, "Ultrafast Dynamics in the Three-Photon, Double-Resonance Ionization of Phenol via the S_2 Electronic State," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 3735-3740 (2001). — 3-Photon Ionization; C_6H_5OH; Channels

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(88804) (1+1) Mode, NO/NO_2 Mixture Monitoring Method Involving Fragmentation — REMPI,NO

(89148) Excited State Source, Supersonic Plasma Jet, REMPI Monitor, Rotationally Cold, T_{vib}=6700 K — REMPI; NO(v≤18)

43. P.E. CURVES/SURFACES/ENERGY LEVELS

(See also Section 26 for Spectral Aspects, Section 39 for Unimolecular Surface Dynamics and Section 40 for Surface Dynamics)

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89030. Schwenke, D.W., "Beyond the Potential Energy Surface: Ab Initio Corrections to the Born-Oppenheimer Approximation for H_2O," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 2352-2360 (2001).

Energy Levels
H_2 ,H_2O
B.-O. Corrections
Magnitudes

89031. Schwenke, D.W., "A First Principle Effective Hamiltonian for Including Nonadiabatic Effects for H_2^+ and HD^+," *J. Chem. Phys.* 114, 1693-1699 (2001).

Vibrational Levels
H_2^+,HD^+
Nonadiabatic
Corrections
Calculations

89032. Chen, R., G. Ma and H. Guo, "Six-Dimensional Quantum Calculations of Highly Excited Vibrational Energy Levels of Hydrogen Peroxide and Its Deuterated Isotopomers," *J. Chem. Phys.* 114, 4763-4774 (2001).

Vibrational
Energy Levels
H_2O_2 ,D_2O_2
HDO_2
≤10,000 cm^{-1}
Calculation
Method

89033. Elbs, M., H. Knockel, T. Laue, C. Samuelis and E. Tiemann, "Observation of the Last Bound Levels Near the Na_2 Ground State Asymptote," *Phys. Rev. A: At. Mol. Opt. Phys.* 59, 3665-3672 (1999).

Energy Levels
Na_2(a,X)
Near Dissociation
Last Bound States
Population Method

89034. Pouchan, C., M. Aouni and D. Begue, "Ab Initio Determination of the Anharmonic Vibrational Spectra of P_2O in the Region 200-2000 cm^{-1}," *Chem. Phys. Lett.* 334, 352-356 (2001).

Vibrational
Energy Levels
P_2O
Calculations
Accuracies

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P.E. Surfaces
Absorption Data
Inversion
Method
Singularity
Problem

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P.E. Curves
AlC,AlC^-
BC,BC^-
Low-lying States
Spectral Constants
D_e

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P.E. Curves
CCl
Low-lying States
Spectral Constants
Calculations

89038. Li, Y., and J.S. Francisco, "CASSCF and MRCI Studies of the Electronic Excited States of CH_2Cl and CH_2Br," *J. Chem. Phys.* 114, 2879-2882 (2001). | P.E. Curves; CH_2Cl; CH_2Br; Low-lying States; Energies; Transitions

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89041. Mebel, A.M., M. Baer, V.M. Rozenbaum and S.H. Lin, "Ab Initio Study of Nonadiabatic Coupling Matrix Elements between Excited $2^2A'$ and $3^2A'$ Electronic States of C_2H," *Chem. Phys. Lett.* 336, 135-142 (2001). | P.E. Surfaces; $C_2H(2^2A',3^2A')$; Conical Intersection; Coupling Elements; Characterization

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(89103) P.E. Surface, IVR, Calculations | C_2H_3Br

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(88865) P.E. Surface Dynamics, HCN Product Energies | c-$C_3H_3N_3 + h\nu$

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P.E. Curves
CdRg(X)
Spectral Constants
D_e
Calculations

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P.E. Curves
CdRg(B,A-X)
Transitions
Spectral Constants
F.C. Factors
Calculations

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P.E. Surfaces
F,Cl+H_2
Long Range
Interactions

89049. Kornweitz, H., and A. Persky, "Three-Center Semiempirical Potential Energy Surfaces for the Reactions F+H_2O and F+OH," *Chem. Phys. Lett.* 331, 132-136 (2000).

P.E. Surfaces
F+H_2O,OH
Construction
Testing

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P.E. Curve
$H^{79}Br$
$v \leq 8$ Levels
Dipole Moment

89051. Kiriyama, F., B.S. Rao and V.K. Nangia, "Electric Dipole Moment Function of $H^{35}Cl$," *J. Quant. Spectrosc. Radiat. Transfer* 69, 35-40 (2001).

P.E. Curve
$H^{35}Cl$
$v \leq 7$ Levels
Dipole Moment

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Potential
Functions
HCl(B,X)
4 Isotopomers
Database
Least Squares Fit

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P.E. Surfaces
HNCO(S_1,S_0)
Conical
Intersections
Mapping

89054. Yu, H.G., and A.J.C. Varandas, "Ab Initio Theoretical Calculation and Potential Energy Surface for Ground State HO_3," *Chem. Phys. Lett.* 334, 173-178 (2001).

P.E. Surface
HO_3
Energies,Barriers

89055. Sanz, C., O. Roncero, C. Tablero, A. Aguado and M. Paniagua, "The Lowest Triplet State $^3A'$ of H_3^+: Global Potential Energy Surface and Vibrational Calculations," *J. Chem. Phys.* 114, 2182-2191 (2001).
P.E. Surface
$H_3^+(^3A')$
Vibrational Levels
Calculations
Accuracies

(88481) P.E. Curves, Rate Constants, Isotopes, Mechanism, Calculations
$He_2^+(v,J) + e^-$

89056. Munro, L.J., J.K. Johnson and K.D, Jordan, "An Interatomic Potential for Mercury Dimer," *J. Chem. Phys.* 114, 5545-5551 (2001).
P.E. Curve
Hg_2
Spectral Constants
D_e, r_e

89057. Rousseau, S., A.R. Allouche and M. Aubert-Frecon, "Theoretical Study of the Electronic Structure of the KRb Molecule," *J. Mol. Spectrosc.* 203, 235-243 (2000).
P.E. Curves
KRb
Low-lying States
Spectral Constants

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P.E. Curve
LiH(D)
B.-O. Breakdown
Assessments

89059. Kerkines, I.S.K., and A. Mavridis, "An Accurate Description of the LiNe($X^2\Sigma^+$,$A^2\Pi$, and $B^2\Sigma^+$) States," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 105, 1983-1987 (2001).
P.E. Curves
LiNe(B,A,X)
Spectral Constants
D_e
Calculations

89060. Hollebeek, T., T.-S. Ho, H. Rabitz and L.B. Harding, "Construction of Reproducing Kernel Hilbert Space Potential Energy Surfaces for the 1A″ and 1A′ States of the Reaction $N(^2D) + H_2$," *J. Chem. Phys.* 114, 3945-3948 (2001).
P.E. Surfaces
$N(^2D) + H_2$
Interpolated
Construction
Method

(88485) Singlet/Triplet P.E. Surfaces, Nonadiabatic Crossing Mechanism Role
$N^+ + NH_3$

89061. Alexander, M.H., P. Soldan, T.G. Wright, Y. Kim, H. Meyer, P.J. Dagdigian and E.P.F. Lee, "The NO($X^2\Pi$)-Ne Complex. II. Investigation of the Lower Bound States Based on New Potential Energy Surfaces," *J. Chem. Phys.* 114, 5588-5597 (2001).
P.E. Surfaces
NO.Ne
Vibrational Levels
IR Spectral
Predictions

(89091) P.E. Surfaces, Structural Calculations, Geometry, Frequencies
NO_3^+

89062. Geum, N., and G.-H. Jeung, "Undulating Potential Curves of the Rydberg States of NaHe," *Chem. Phys. Lett.* 333, 314-318 (2001).
P.E. Curves
NaHe
Rydberg States
10 $^2\Sigma^+$ States
Shapes

89063. Pashov, A., W. Jastrzebski, W. Jasniecki, V. Bednarska and P. Kowalczyk, "Accurate Potential Curve for the Double Minimum $2^1\Sigma_u^+$ State of Na_2," *J. Mol. Spectrosc.* 203, 264-267 (2000).

P.E. Curve
$Na_2(2^1\Sigma_u^+)$
Polarization
Labeling Spectrum
Constants

89064. Hoffman, G.J., and M. Colletto, "An ab Initio Study of Some Noble Gas Monohalides," *J. Chem. Phys.* 114, 2219-2227 (2001).

P.E. Curves
NeF,ArF,KrF
XeF,XeCl
Spectral Constants
T_e ,D_e
Accuracies

89065. Minaev, B.F., and V.A. Minaeva, "MCSCF Response Calculations of the Excited States Properties of the O_2 Molecule and a Part of Its Spectrum," *Phys. Chem. Chem. Phys.* 3, 720-729 (2001).

P.E. Curves
O_2
8 Low-lying States
Spectral Constants
Avoided Crossing
(f-X) Transition
Moment

89066. Ornellas, F.R., "Theoretical Spectroscopic Characterization of the $B^2\Sigma^+$ State of SiP and of the ($B^2\Sigma^+$-$X^2\Pi$) and ($B^2\Sigma^+$-$A^2\Sigma^+$) Transitions," *Chem. Phys. Lett.* 335, 420-426 (2001).

P.E. Curves
SiP
Low-lying States
B-State Lifetime
Spectral Constants

89067. Czuchaj, E., and M. Krosnicki, "CCSD(T) Calculation of the Ground State Potential Curves for the Zn-Rare Gas van der Waals Molecules," *Chem. Phys. Lett.* 335, 440-448 (2001).

P.E. Curves
ZnRg(X)
Spectral Constants

44. ATOMIC/MOLECULAR STRUCTURES

(See also Section 26 for Spectrally Measured Structures)

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Stretching
Force Constant/
r_e Correlation
Badger's Rule
Accuracy
Assessment

89069. Burns, K.L., D. Bellert, A.W.-K. Leung and W.H. Breckenridge, "The Effects of Dispersive C_n/R^n Attraction on M^+/Rg Bonding (M^+=Atomic Metal Ion, Rg=Rare Gas Atom)," *J. Chem. Phys.* 114, 2996-3002 (2001).

Structural
Bonding
M^+Rg
Model Potential
Analysis

89070. Panek, J., and Z. Latajka, "A Theoretical Study of NO_2 Complexes with Aluminum and Gallium Based on Topological Analysis of Electron Density and Electron Localization Function," *Chem. Phys. Lett.* 332, 617-623 (2000).

Structural Calculations
$AlNO_2$, $GaNO_2$
Geometries
Frequencies
Binding

89071. Petrie, S., "Group IIIA Metal Dihalide Ions: Identification of a Possible New Class of Associative Ionization Reactions," *Int. J. Mass Spectrom. Ion Process.* 184, 191-199 (1999).

Structural Calculations
MXY^+
M=B,Al,Ga
X,Y=F,Cl,Br
Geometries
ΔH_f, IPs
Chemi-ionization Channels

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$(MX)_2$
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X=F,Cl
Geometries
Frequencies
Stabilities

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CH_2N, CH_2P
Geometries
Frequencies
Low-lying States
Energies

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CH_2NO_2
Isomers
Relative Energies
Experimental
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CH_4P_2
Isomers
Geometries
Energies

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CN_2
Isomers
Geometries
Frequencies
IPS

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CO^-
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Energies

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CF_2XCF_2X
CF_2XCF_2
X=Cl,Br,I
Geometries
Stabilities

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CCN(C,B,A,a,X)
CNC(B,A,X)
CNN($1^1\Pi$,A,b,a,X)
NCN(A,b,a,X)
Geometries
Spectral Constants
Energies

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Excited ^{1}States
Energies
Transitions

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Geometries
Frequencies
(A-X) Synthetic Spectrum

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Geometries

Energies
Spectral Transitions

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CuO_2
Geometries
Frequencies
Energies

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Cu_2 ,Ag_2 ,Au_2
Spectral Constants
D_e
DFT Method

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M=La,Lu,Ac,Lr
Spectral Constants
D_0

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Ionic Bond
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Rotational
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Isomers
Geometries
Frequencies
IR Intensities

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NO_2^+
Geometries
Frequencies

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NO_3^+
Geometry
Frequencies
P.E. Surfaces

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O_4^-
Dissociation Channels

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SiCH(A,X)
Geometries
Frequencies
Energies

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SiH_3O^-
Geometries
Frequencies
PA

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TlH(X)
Spectral Constants
D_e

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VO_n, VO_n^+
Geometries

Frequencies
Excited States
Relative
Stabilities

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V_3,V_3^+
Geometries
Frequencies
PFI-ZEKE
Synthetic Spectrum

45. ENERGY TRANSFER

(See also Section 27 for Electronically Excited State Relaxation Processes)

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E-E Transfer
Conformational
States
LIF Decays
Rate Constants
Method

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E-V,V-V
Energy Pumping

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Energy Transfer
Li(3^2D)+Ne,Ar
Rate Constants
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Na.H_2+hν
E-V Transfer

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Effects
LIF
Resonance Raman
Pulsed Excitation
Theory

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DCO^+(ν_{CO})
Radiative Lifetimes
Measurement
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CO_2 Formation
Mechanism
Measurements

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P.E. Surface
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c-$C_4H_{4-n}N_2(CH_3)_n$
He,Ar,Kr Quenching
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Energy Transfer
c-C_7H_{10}
C_7H_{15}
Polyatomics
Overview

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HD+He
Rate Constants
v=1 Quenching
Rates

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Relaxation
HF(v)+Ar
HCl(v)+Ar
Interaction
Anisotropy
Product High J

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Rate Constants
Channels

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(88651)	50 Molecules, Diatomics, Spectral Constants, Calculation Method	D_e
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$\Delta H_f(IO_2)$
Photoionization
Spectral
Measurements

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CCl_2, CCBr, CBr_2
Ion/Molecule
Acidities
Measurements

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Bending Frequency
Photoionization
Spectrum

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CF,CCl,CH
Dissociation
Measurements
$CHCl^-$, $CFCl^-$, CCl_2^-

(88662) Threshold Photoelectron Spectra, $CH_2F_2^+$, $CF_2Cl_2^+$, $CF_2Br_2^+$, Fragmentation

$\Delta H_f(CF_2Br^+, CHF_2^+)$

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Calculations

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$IP(CN_2)$

(88931) $C+N_2$, $N+CN$ Reaction Energetics, Calculations

ΔH_f(CNN,NCN)

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$D(^{13}CO)$

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CP,PCP,PCCP
$CP^+(X^3\Pi)$
Calculations

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Spectral Constants
Calculations
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ΔH_f
Measurements

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(88744) $Co^+(^5F,^3F)+H_2O$ Reactive Channels, Energies — $D_0(CoH^+,CoO^+)$

(89085) Structural Calculations, Spectral Constants, DFT Method — $D_e(Cu_2,Ag_2,Au_2)$

(88893) $D_2S+h\nu$ Photodissociation, D, SD(A) Product Energies, Measurements — $D_0(D_2S)$

(88848) GeH_2+SiH_4 Rate Constants, Temperature Dependence, RRKM Modeling — $\Delta H_f(GeH_2)$

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(89086) M=La, Lu, Ac, Lr, Structural Calculations, Spectral Constants — $D_0(MF,MH,MO)$

(88692) Absorption/LIF, Dunham Coefficients, Measurements — $D_e(LiAr(B,A))$

(89059) P.E. Curves, Spectral Constants, Calculations — $D_e(LiNe(B,A,X))$

(88484) Mg Flame Chemistry, Ions/Neutrals, Rate Constants, Mass Analysis — $D_0(MgO,MgOH)$
$D_0(MgOH^+,Mg(OH)_2)$

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